Fredholm determinants for the stability of travelling waves

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Abstract

This thesis investigates both theoretically and numerically the stability of travelling wave solutions using Fredholm determinants, on the real line. We identify a class of travelling wave problems for which the corresponding integral operators are of trace class. Based on the geometrical interpretation of the Evans function, we give an alternative proof connecting it to (modified) Fredholm determinants. We then extend that connection to the case of front waves by constructing an appropriate integral operator. In the context of numerical evaluation of Fredholm determinants, we prove the uniform convergence associated with the modified/regularised Fredholm determinants which generalises Bornemann's result on this topic. Unlike in Bornemann's result, we do not assume continuity but only integrability with respect to the second argument of the kernel functions. In support to our theory, we present some numerical results. We show how to compute higher order determinants numerically, in particular for integral operators belonging to classes $\mathfrak{I}_3$ and $\mathfrak{I}_4$ of the Schatten–von Neumann set. Finally, we numerically compute Fredholm determinants for some travelling wave problems e.g. the 'good' Boussinesq equation and the fifth-order KdV equation.

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Chapter 1

Introduction

1.1 Introduction

In nature we often observe coherent structures. These include localised objects such as atoms or molecules, or light pulses propagating along optical fibres, and so forth. To understand these natural processes, one is often required to develop a mathematical model in which the observed phenomena are among the solutions to that model. Of particular interest to us are travelling waves, these are steady/stationary solutions to models such as those for chemical reactions (reaction-diffusion equation), quantum states (Schrödinger equation) and so forth. For these solutions to represent the observed phenomena, they must be stable, in particular, linearly stable. By this we mean that, if we perturb the travelling waves a little bit and if they settle back to the original form with time, then they are stable and we are likely to observe them in nature since they will have some permanence. If not, they are unstable and we are unlikely ever to see them. By linearising the nonlinear differential operator associated with the model about its stationary solution, the stability analysis of travelling waves is reduced to computing eigenvalues associated with a linear differential operator. Typically under suitable conditions and in the one dimensional case particularly, these eigenvalues are inferred from a system of algebraic equations obtained by some discretisation method like finite differences and Galerkin methods. In our case, the essential spectrum associated with the linear differential operator is not empty. Therefore in the case of finite differences, one needs to increase the size of the system of algebraic equations in order to track the isolated non-moving points (eigenvalues)

in the complex plane. Over the last half century, another competitive method has emerged for such a purpose. This method computes the zeros of an analytic function which is similar in construction to the characteristic polynomial for finite dimensional matrices. More precisely, the analytic function, introduced by J.W. Evans [23] in his study on the stability of nerve axons, is the determinant of the set of solutions associated with the eigenvalue problem. We will call this function the *Evans function*. Others communities call *m-function* or Weyl-Titchmarsh function or *miss-distance function* [53]. A more precise definition of the Evans function was introduced in [1]. This definition, based on the exterior algebra framework, measures if whether the subspaces decaying at infinity associated with the eigenvalue problem intersect or not. The first numerical computation of the Evans function goes back to Evans himself where he dealt with one dimensional subspace that decays at either plus/minus infinity (see also [56]). Unfortunately if both subspaces are of dimension greater than one, then numerical problems arise due to different exponentially growing/decaying solutions (the spanning vectors of the subspaces decaying at infinity) associated with the problem. Lifting the problem into the exterior algebra framework resolves these numerical problems, since the subspaces decaying at infinity correspond to a single subspace in the exterior system (cf. [2], [14], [13], [45], [26], [9]). However the dimension of the lifted problem increases exponentially with the order of the problem. To circumvent this, methods such as continuous orthogonalisation [40] or Grassmannian-shooting [52] are employed.

The approach taken in this thesis is a very different one as it is based on computing the zeros of the *Fredholm determinant*. The Fredholm determinant, introduced by Fredholm [24], is an entire function of the spectral parameter which characterises the solvability of what are called Fredholm integral equations of the second kind. In order to derive the Fredholm determinant, Fredholm assumed that the kernel function associated with the integral operator is continuous in both arguments over a finite interval of the real line. Using the rectangular rule to approximate the integral operator, he replaced the integral equations by a system of algebraic equations whose determinant was then computed as the rectangles width goes to zero. The convergence of the scheme was proved by Hilbert [37] and then was generalised by Bornemann [10]

for any quadrature rule (e.g. Gaussian quadrature) which converges for continuous functions. Hilbert [37] relaxed the continuity ansatz of the kernel assumed by Fredholm, and considered kernel functions that are square integrable. He observed that in order to achieve convergence of the determinant it suffices to set the diagonal elements of the kernel to zero. The development of the theory of integral equations with square integrable kernels was also conducted by Calerman [15], Smithies [68], Plemelj [58] and others, and the generalisation to other than square integrable kernel functions is given by Gohberg and Krein [33] and Dunford and Schwartz [20], for example. This generalisation of the Fredholm determinant led to what are called *regularised* or *modified Fredholm determinants*. Under this generalisation, the Fredholm determinant is then given as the determinant of a trace class perturbation of the identity operator, for integral operators with continuous kernels in particular. Among the applications of Fredholm determinants, we cite for example from mathematical physics [66], [25], [46], [42], [28] and [29] where the authors used the Fredholm determinant to compute eigenvalues or resonances associated with Schrödinger problems.

1.2 Motivation and aim

Like the Evans function, the zeros of Fredholm determinant coincide in location and multiplicity with eigenvalues of the underlying integral operator. Therefore, we aim to reformulate the linear differential eigenvalue problem into an integral equations and then compute the corresponding eigenvalues. What motivate us to pursue this direction is the following:

- To our knowledge, no has numerically computated the Fredholm determinant associated with the linear stability of travelling waves.
- The natural extension of (modified) Fredholm determinants to higher dimensional problem.
- In [27], [30], [66] and [46], the authors have established the connection between the Fredholm determinant and the Evans function.
- Bornemann [10] proved the exponential convergence when computing the Fredholm determinant for smooth kernel functions.

The last two items suggest that if the kernel of the corresponding integral is smooth, then computing the Fredholm determinant might be a better option than the Evans function.

1.3 Contribution

Although the connection between the Fredholm determinant and the Evans function has been already established by B. Simon [66] and Gesztesy et al. [27], our approach to achieve this result is different. For clarity, the connection found in [27] relies on the fact that the kernel of the integral operator is semi-separable. Hence a decomposition into a finite rank and a Volterra operator is available. This yields a reduction of the infinite determinant to a finite dimensional one. To reduce the Fredholm determinant to the Evans function through the latter finite dimensional determinant, a first order system of differential equations is introduced. The determinant of the fundamental matrix solution corresponding to the system coincides with the finite dimensional determinant (Fredholm determinant). Our approach is rather geometrical. That is, if the unstable subspace (the subspace decaying at $-\infty$) is orthogonal to a given stable subspace (the subspace decaying at $+\infty$) defined by the set of solutions of the adjoint problem, then necessary we must have that the stable and the unstable subspaces intersect. This is because the unstable subspace and that of the adjoint problem are orthogonal. To measure the orthogonality condition of subspaces, we introduce a finite dimensional matrix whose determinant is equal to the Fredholm determinant. It turns out that this determinant is nothing other than the determinant of a block matrix of the matrix defining the Evans function. Hence our finite dimensional determinant (Fredholm determinant) is equal to the Evans function, up to a nonvanishing analytic function. As noted in our approach:

- The semi-separability property of the kernel function is not needed;
- Our approach enables us to directly extend the connection between the Evans function and the Fredholm determinants associated with other than trace class or Hilbert–Schmidt operators;
- The finite dimensional determinant that we have introduced is, in fact, equal to the determinant of the fundamental matrix solution given in [27] and [30].

Hence the determinant of the fundamental matrix solution has a geometrical interpretation which, in our opinion, was not clear in [27].

We remark that our relation connecting the Fredholm determinant and the Evans function translates the method used in [40] and [52] to avoid the numerical stiffness in computing the Evans function, in some sense. Indeed, the nonvanishing analytic function in our relation corresponds to the extraction of different exponentially growing/decaying solutions associated with the problem. Therefore by analogy to the method of [40] and [52], the other function (Fredholm determinant in our case) given in the relation connecting the Evans function is the one which is numerically stable. As further contributions, we have identified a class of travelling wave problem for which the corresponding integral operators are of trace class. Moreover, we have constructed the Fredholm determinant for front waves.

In the context of computing the Fredholm determinant, we have extended Bornemann's result on the uniform convergence of Fredholm determinants associated with continuous kernels to those that are Lebesgue integrable with respect to the second argument. Moreover, we showed how to (numerically) compute the p-modified Fredholm determinants, in particular for $p = 3, 4$.

For the numerical evaluation of Fredholm determinants associated with the linear stability of travelling waves, we numerically investigated the accuracy and the performance in computing the zeros of Fredholm determinants and that of Evans function.

1.4 Organisation of the thesis

The organisation of the thesis is as follows. In Chapter 2, we recall some properties about compact operators and the p-regularised Fredholm determinants that we shall use throughout the thesis. In Chapter 3, we introduce the Evans function as well as its different constructions. Chapter 4 is aimed at showing the connection between the Evans function and the Fredholm determinants associated with pulse and front waves. Also, we identify a class of eigenvalue problems for which the associated integral operators are of trace class. In Chapter 5, we discuss the numerical evaluation of

the p-modified Fredholm determinants. We show the uniform convergence associated with any operator in the Schatten–von Neumann class. Additionally, we demonstrate how to compute higher order Fredholm determinants. In Chapter 6, we numerically compute the Fredholm determinant for a class of travelling wave problems. We then compare the error in computing eigenvalues (zeros) by the Evans function and the Fredholm determinant approaches.

Chapter 2

Compact operators and Fredholm determinants

In this chapter, we recall some basic material about compact operators and the regularised Fredholm determinants. Throughout this thesis, $\mathbb{H}$ is the Hilbert space with inner-product $\langle \cdot, \cdot \rangle$. Typically, $\mathbb{H}$ will be separable, but it will not be assumed until it is needed. When dealing with integrals, $\mathbb{H} = L^2$.

2.1 Fredholm determinants

In this section, we briefly recall the construction of the Fredholm determinant as given in the book of Riesz and Sz.-Nagy [63]. Fredholm in [24] was interested in solving, for all $x \in [a, b] \subset \mathbb{R}$, the following equation

$$f(x) + z \int_a^b k(x, y) f(y) \mathrm{d}y = g(x), \tag{2.1}$$

where f is the unknown, $z \in \mathbb{C}$ is a given parameter, and the nonzero functions g and k are assumed to be continuous on $[a, b]$ and $[a, b]^2$, respectively. Approximating the integral in (2.1) by the rectangular rule yields the system of linear algebraic equations

$$f_i + zh \sum_{j=1}^{n} k_{ij} f_j = g_i, \quad (i, j = 1, \ldots, n), \tag{2.2}$$

where $f_i = f(x_i),\ k_{ij} = k(x_i, y_j),\ g_i = g(x_i)$ and $h = (b-a)/n$ with $x_i = a + ih$ and $y_j = a + jh$. Thus equation (2.2) is solvable depending on whether the determinant

$$P_n(z) = \det \begin{pmatrix} 1 + zhk_{11} & zhk_{12} & \cdots & zhk_{1n} \\ zhk_{21} & 1 + zhk_{22} & \cdots & zhk_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ zhk_{n1} & zhk_{n2} & \cdots & 1 + zhk_{nn} \end{pmatrix} \tag{2.3}$$

is zero or not. Since $P_n(z)$ is a polynomial in z, equation (2.2) has a unique solution for all values of z except for at most a finite number of values (eigenvalues). Taking the limit as n goes to infinity of $P_n(z)$ results in the entire function (a non-obvious computation see [63])

$$d(z) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_a^b \cdots \int_a^b \det(k(x_p, x_q))_{p,q=1}^n \mathrm{d}x_1 \cdots \mathrm{d}x_n \tag{2.4}$$

called the *Fredholm determinant*. The series in (2.4) converges for all $z \in \mathbb{C}$ (see [63]). This follows by applying Hadamard inequality[1].

Let $\mathbb{D}$ be the space of integral operators with continuous kernels acting on $C[a, b]$, the space of continuous functions in $[a, b]$, and let $\mathbb{D}^{n\times n}$ be the space of matrices with entries from $\mathbb{D}$ see [32, Sec. VI.1.1]. Then for systems of integral equations, we have the following:

Theorem 2.1 (Gohberg et al. [32, Chap. VI, p. 128])**.** *Let $\mathcal{K}_{jm}$ be integral operators with continuous kernels $k_{jm}(x, y)$ $(a \leqslant x, y \leqslant b)$, $\mathcal{K} = (\mathcal{K}_{jm})_{j,m=1}^N \in \mathbb{D}^{N\times N}$ and let*

$$\det_{\mathbb{D}^{N\times N}}(\mathrm{id} + z\mathcal{K}) = 1 + \sum_{n=1}^{\infty} \frac{c_n(\mathcal{K})}{n!} z^n. \tag{2.5}$$

The $c_n(\mathcal{K})$ are given by

$$c_n(\mathcal{K}) = \sum_{i_1, i_2, \ldots, i_n = 1}^{N} \int_a^b \cdots \int_a^b \det\big(k_{i_p i_q}(x_p, x_q)\big)_{p,q=1}^n \mathrm{d}x_1 \cdots \mathrm{d}x_n. \tag{2.6}$$

[1]If the entries a_{ij} of an $n \times n$ matrix A satisfy $|a_{ij}| \leqslant M$ for all i, j, then $|\det(A)| \leqslant M^n n^{n/2}$, for some constant $M > 0$.

In particular, we see

$$c_1(\mathcal{K}) = \sum_{i=1}^{N} \int_a^b k_{ii}(x,x)\mathrm{d}x = \sum_{i=1}^{N} \operatorname{tr} \mathcal{K}_{ii} = \operatorname{tr} \mathcal{K}, \tag{2.7}$$

where $\operatorname{tr} \mathcal{K}$ *denote the trace of* $\mathcal{K}$ *(see subsection 2.3.1 ahead).*

(2.5) defines the Fredholm determinant for a system of integral equations and converges for all $z \in \mathbb{C}$ (see [32]). Note that when $N = 1$ (the scalar case), the Fredholm determinant in (2.5) reduces to that given in (2.4). If $k(x,x) \notin L^1\big((a,b)\big)$, both series in (2.6) and (2.4) might not converge. However Hilbert [37] (see also [10] and [67]) observed that, in order to get convergence for square-integrable kernels ($k \in L^2\big((a,b)^2\big)$), it suffices to redefine the kernel as follows

$$\tilde{k}(x,y) = \begin{cases} 0, & \text{if } x = y \\ k(x,y), & \text{otherwise.} \end{cases}$$

In this case (square integrability), the *modified Fredholm determinant*

$$d_2(z) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_a^b \cdots \int_a^b \det(\tilde{k}(x_p, x_q))_{p,q=1}^{n} \mathrm{d}x_1 \cdots \mathrm{d}x_n \tag{2.8}$$

converges for all $z \in \mathbb{C}$.

For a system of integral equations, if the series

$$\operatorname{tr} \mathcal{K}_{mm} \coloneqq \sum_{n=1}^{\infty} \langle u_n, \mathcal{K}_{mm} u_n \rangle$$

converges for any independent orthonormal basis $\{u_n\}_{n \geqslant 1}$ of $L^2\big((a,b)\big)$ and $\mathcal{K}_{mm}$ are Hilbert–Schmidt operators, Gohberg et al. [32, Theorem 6.2, p. 131] have defined the following

$$\tilde{k}_{jm}(x,y) = \begin{cases} \dfrac{1}{b-a} \operatorname{tr} \mathcal{K}_{mm}, & \text{if } x = y \text{ and } i = j \\ k_{jm}(x,y), & \text{otherwise.} \end{cases}$$

Note that if $b - a = \infty$ or if the above infinite sum does not converge, the diagonal elements of the matrix-valued function $\tilde{k}_{jm}(x,y)$ are set to zero.

2.2 Bounded operators

Most of the results in this section are collected from Reed and Simon [60].

Definition 2.1. A bounded linear operator from a Banach space $(E, \|\cdot\|_1)$ to Banach space $(F, \|\cdot\|_2)$ is a function $\mathcal{K}\colon E \to F$ which satisfies, for all $u_1, u_2 \in E$ and $\alpha, \beta \in \mathbb{C}$,

1. $\mathcal{K}(\alpha u_1 + \beta u_2) = \alpha \mathcal{K} u_1 + \beta \mathcal{K} u_2$;

2. For some $C \geqslant 0$, $\|\mathcal{K} u_1\|_2 \leqslant C \|u_1\|_1$.

The *operator norm* is then given by

$$\|\mathcal{K}\| = \sup_{u \neq 0} \frac{\|\mathcal{K} u\|_2}{\|u\|_1} \tag{2.9}$$

Let $\mathbb{B}(E, F)$ denote the set of bounded operators from E onto F. We write $\mathbb{B}(E) = \mathbb{B}(E, E)$. In what follows, $\mathbb{H}_i$ are Hilbert spaces, for $i = 1, 2$.

Definition 2.2 (Positive operator)**.** An operator $\mathcal{K} \in \mathbb{B}(\mathbb{H})$ is called *positive* if $\langle \mathcal{K} u, u \rangle \geqslant 0$ for all $u \in \mathbb{H}$. We write $\mathcal{K} \geqslant 0$ for such an operator and, for example, $\mathcal{K}_1 \leqslant \mathcal{K}_2$ if $\mathcal{K}_2 - \mathcal{K}_1 \geqslant 0$.

Note that every bounded positive operator on $\mathbb{H}$ is self-adjoint: $\mathcal{K}^* = \mathcal{K}$. For any $\mathcal{K} \geqslant 0$ there is a unique operator $\sqrt{\mathcal{K}}$ such that $\mathcal{K} = (\sqrt{\mathcal{K}})^2$. For any $\mathcal{K} \in \mathbb{B}(\mathbb{H})$, note that $\mathcal{K}^* \mathcal{K} \geqslant 0$ since $\langle \mathcal{K}^* \mathcal{K} u, u \rangle = \|\mathcal{K} u\|_{\mathbb{H}}^2 \geqslant 0$. In particular, we define $|\mathcal{K}| = \sqrt{\mathcal{K}^* \mathcal{K}}$. Lastly note that $\||\mathcal{K}| u\|_{\mathbb{H}}^2 = \|\mathcal{K} u\|_{\mathbb{H}}^2$.

Definition 2.3 (The resolvent)**.** Let $\mathcal{K} \in \mathbb{B}(\mathbb{H})$. A complex number λ is in the *resolvent set* $\rho(\mathcal{K})$ of $\mathcal{K}$ if $\mathcal{K} - \lambda \mathrm{id}$ is a bijection with a bounded inverse.

Definition 2.4 (The spectrum)**.** Let $\mathcal{K} \in \mathbb{B}(\mathbb{H})$. Then

1. Any complex number $\lambda \notin \rho(\mathcal{K})$ is said to be in the *spectrum* $\sigma(\mathcal{K})$ of $\mathcal{K}$;

2. The set of $\lambda \in \sigma(\mathcal{K})$ for which $\mathcal{K} - \lambda \mathrm{id}$ is not injective is called the *point spectrum* of $\mathcal{K}$ and is denoted by $\sigma_p(\mathcal{K})$. Every number $\lambda \in \sigma_p(\mathcal{K})$ is called an *eigenvalue* of $\mathcal{K}$, and every function $u \neq 0$ with $(\mathcal{K} - \lambda \mathrm{id}) u = 0$ for $\lambda \in \sigma_p(\mathcal{K})$ is called an *eigenfunction* of $\mathcal{K}$.

2.3 Compact operators

Definition 2.5 (Reed and Simon [60])**.** A bounded operator $\mathcal{K} \in \mathbb{B}(\mathbb{H}_1, \mathbb{H}_2)$ is *compact* (or completely continuous) if $\mathcal{K}$ takes bounded sets in $\mathbb{H}_1$ into precompact sets in $\mathbb{H}_2$. Equivalently, $\mathcal{K}$ is compact if and only if for every bounded sequence $\{x_n\}_{n=1}^{\infty} \subset \mathbb{H}_1$, $\{\mathcal{K}x_n\}$ has a subsequence convergent in $\mathbb{H}_2$.

Let the set of compact operators from $\mathbb{H}_1$ onto $\mathbb{H}_2$ be denoted by $\mathfrak{I}_\infty(\mathbb{H}_1, \mathbb{H}_2)$, and write $\mathfrak{I}_\infty = \mathfrak{I}_\infty(\mathbb{H}, \mathbb{H})$.

Definition 2.6 (Singular value)**.** Let $\mathcal{K} \in \mathfrak{I}_\infty$ and $|\mathcal{K}|$ its associated positive operator. Then any number $\mu \in \sigma_p(|\mathcal{K}|)$ is called *singular value* of $\mathcal{K}$ or eigenvalue of the operator $|\mathcal{K}|$.

Theorem 2.2 (Reed and Simon [60])**.** *Let $\mathcal{K} \in \mathfrak{I}_\infty$. Then there exist (not necessarily complete) orthonormal sets $\{u_n\}_{n\geqslant 1}$ and $\{v_n\}_{n\geqslant 1}$ and positive real numbers $\{\mu_n\}_{n\geqslant 1}$ (singular values) so that*

$$\mathcal{K} = \sum_{n=1}^{\infty} \mu_n \langle u_n, \cdot \rangle v_n.$$

Theorem 2.3 (Reed and Simon [60])**.** *Let $\mathcal{K} \in \mathfrak{I}_\infty$. Then the spectrum of $\mathcal{K}$, $\sigma(\mathcal{K})$ is a discret set having no limit points except perhaps $\lambda = 0$. Further, any nonzero $\lambda \in \sigma(\mathcal{K})$ is an eigenvalue and the corresponding space of eigenfunctions is finite dimensional (geometric multiplicity).*

The above theorem simply means that if $\mathcal{K} \in \mathfrak{I}_\infty$ then the spectrum of $\mathcal{K}$ consist of nonzero eigenvalues $\sigma_p(\mathcal{K})$ and a possible accumulation point at the origin. Thus, the compactness property of an operator guarantees that either $(\mathrm{id} - \mathcal{K})^{-1}$ exists or $\mathcal{K}u = u$ has nontrivial solution (Fredholm alternative).

Theorem 2.4 (Reed and Simon [60])**.** *Let $\mathbb{H}$ be a separable Hilbert space. Then every compact operator on $\mathbb{H}$ is the norm limit of a sequence of operators of finite rank.*

The above theorem means that the closure in the operator norm of the set of finite rank operators in $\mathbb{B}(\mathbb{H})$ is the set of compact operators (the approximation property). That is, the approximation property holds in a separable Hilbert space. If $\dim \mathbb{H} < \infty$, then any bounded operator $\mathcal{K} \in \mathbb{B}(\mathbb{H})$ is finite rank and hence compact.

Theorem 2.5 (Reed and Simon [60])**.** *Let $\mathcal{K}_1, \mathcal{K}_2 \in \mathbb{B}(\mathbb{H})$. Then*

1. *If* $\{\mathcal{K}_n\}_{n\geqslant 1}$ *are compact and* $\mathcal{K}_n \to \mathcal{K}_1$ *in the operator norm, then* $\mathcal{K}_1$ *is compact;*

2. $\mathcal{K}_1$ *is compact if and only if its adjoint* $\mathcal{K}_1^*$ *is compact;*

3. *If* $\mathcal{K}_1$ (or $\mathcal{K}_2$) *is compact then* $\mathcal{K}_1\mathcal{K}_2$ (or $\mathcal{K}_2\mathcal{K}_1$) *is compact.*

Two important classes of compact operators that we shall consider in this thesis are the trace class and the Hilbert–Schmidt operators. In the next two subsections, we only give properties which are specific to trace class and Hilbert–Schmidt operators.

2.3.1 Trace class operators

Definition 2.7. Let $\mathbb{H}$ be a separable Hilbert space with orthonormal basis $\{u_m\}_{m=1}^{\infty}$. Then for any positive operator $\mathcal{K} \in \mathbb{B}(\mathbb{H})$, we define

$$\operatorname{tr}\mathcal{K} \coloneqq \sum_{m=1}^{\infty} \langle u_m, \mathcal{K}u_m\rangle,$$

where $\operatorname{tr}\mathcal{K}$ (see Definition 2.9) is independent of the orthonormal basis chosen.

The trace has the following properties:

1. $\operatorname{tr}(\mathcal{K}_1 + \mathcal{K}_2) = \operatorname{tr}\mathcal{K}_1 + \operatorname{tr}\mathcal{K}_2$;

2. $\operatorname{tr}(z\mathcal{K}_1) = \bar{z}\operatorname{tr}\mathcal{K}_1$, for all $z \in \mathbb{C} \setminus \{0\}$;

3. $\operatorname{tr}(U\mathcal{K}_1U^{-1}) = \operatorname{tr}\mathcal{K}_1$ for any unitary operator U;

4. If $0 \leqslant \mathcal{K}_1 \leqslant \mathcal{K}_2$, then $\operatorname{tr}\mathcal{K}_1 \leqslant \operatorname{tr}\mathcal{K}_2$.

Definition 2.8 (Trace class)**.** An operator $\mathcal{K} \in \mathbb{B}(\mathbb{H})$ is called *trace class* if and only if $\operatorname{tr}|\mathcal{K}| < \infty$. The family of all trace class operators is denoted $\mathfrak{I}_1 = \mathfrak{I}_1(\mathbb{H})$.

Definition 2.9 (Reed and Simon [60])**.** The map $\operatorname{tr}\colon \mathfrak{I}_1 \to \mathbb{C}$ given by $\sum\limits_{n\geqslant 1}\langle u_m, \mathcal{K}u_m\rangle$ where $\{u_m\}$ is any orthonormal basis is called the *trace*.

Theorem 2.6 (Reed and Simon [60])**.** *If* $\mathcal{K} \in \mathfrak{I}_1$ *and* $\{u_m\}_{m=1}^{\infty}$ *is any orthonormal basis, then* $\operatorname{tr}\mathcal{K}$ *converges absolutely and the limit is independent of the choice of basis.*

Suppose that $\mathcal{K}$ is a trace class operator. Then we have (Lidskii's Theorem [65])

$$\operatorname{tr}\mathcal{K} = \sum_{n=1}^{\infty} \lambda_n, \tag{2.10}$$

where $\{\lambda_n\}_{n\geqslant 1}$ are the eigenvalues of the operator $\mathcal{K}$. In fact, the above infinite sum converges absolutely. Then the infinite product $\prod_{n=1}^{\infty}(1+\lambda_n)$ converges [2] (see [65]). Therefore one can define the determinant of $\mathrm{id}+z\mathcal{K}$ (cf. [67], for all $z\in\mathbb{C}$, by

$$\prod_{n=1}^{\infty}(1+z\lambda_n). \tag{2.11}$$

Remark 2.1. 1. In particular if $\mathcal{K}\in\mathfrak{I}_1$ is an integral operator with continuous kernel, then the Fredholm determinant $d(z)$ is equal to (2.11), i.e.

$$d(z)=\prod_{n=1}^{\infty}(1+z\lambda_n). \tag{2.12}$$

2. The Fredholm determinant $d(z)$ (cf. (2.4)) makes sense independently of whether the integral operator $\mathcal{K}$ with continuous kernel is of trace class or not. That is, suppose that the integral operator $\mathcal{K}$ with continuous kernel is not of trace class, then the infinite product in (2.11) will not necessarily converge. Consequently equality (2.12) will not make sense though the Fredholm determinant $d(z)$ is well defined, for all $z\in\mathbb{C}$.

Let $\mathcal{K}$ be an integral operator acting on the Hilbert space $L^2\big((a,b)\big)$, defined for all $x\in[a,b]\subset\mathbb{R}$ by

$$\mathcal{K}u(x)=\int_a^b k(x,y)u(y)\mathrm{d}y,$$

where $k(x,y)$ is continuous on $[a,b]\times[a,b]$. If $\mathcal{K}$ is of trace class, then

$$\mathrm{tr}\,\mathcal{K}=\int_a^b k(x,x)\mathrm{d}x. \tag{2.13}$$

Unfortunately, the converse of this statement is not true. That is, only the continuity of the kernel does not imply that the corresponding integral operator is of trace class. Hence, equality (2.13) might not make sense [3] since $\mathrm{tr}\,\mathcal{K}$ might not converge. An example of such an operator was discovered by Calerman (see Gohberg et al. [32]). Fortunately, each of the following conditions is sufficient to define trace class operator (see Bornemann [10]):

[2] $\prod_{n=1}^{\infty}(1+a_n)$ converges if and only if $\sum_{n=1}^{\infty}|a_n|<\infty$

[3] $\int_a^b k(x,x)\mathrm{d}x$ is finite but $\mathrm{tr}\,\mathcal{K}$ can diverge.

1. If the continuous kernel, k can be represented in the form

$$k(x,y) = \int_c^d k_1(x,z)k_2(z,y)\mathrm{d}z, \quad (x,y \in [a,b])$$

with $k_1 \in L^2\big([a,b]\times[c,d]\big)$ and $k_2 \in L^2\big([c,d]\times[a,b]\big)$;

2. If the kernel $k(x,y)$ is smooth on $[a,b]\times[a,b]$;

3. If the continuous Hermitian[4] kernel $k(x,y)$ satisfies, for all $x, y_1, y_2 \in [a,b]$ and $\alpha > 1/2$, the following inequality

$$|k(x,y_1) - k(x,y_2)| \leqslant c|y_1 - y_2|^\alpha.$$

4. If $\mathcal{K}$ is self-adjoint, positive semidefinite operator with a continuous kernel.

2.3.2 Hilbert–Schmidt operators

Definition 2.10 (Hilbert–Schmidt operator)**.** An operator $\mathcal{K} \in \mathbb{B}(\mathbb{H})$ is called *Hilbert–Schmidt* if $\operatorname{tr}|\mathcal{K}|^2 < \infty$. The family of Hilbert–Schmidt operators is denoted $\mathfrak{I}_2 = \mathfrak{I}_2(\mathbb{H})$.

The space $\mathfrak{I}_2$ with the inner-product

$$\langle \mathcal{K}_1, \mathcal{K}_2\rangle_{\mathfrak{I}_2} \coloneqq \sum_{n=1}^{\infty}\langle \mathcal{K}_1 u_n, \mathcal{K}_2 u_n\rangle, \tag{2.14}$$

where $\{u_n\}_{n\geqslant 1}$ is any orthonormal basis of $\mathbb{H}$ and $\mathcal{K}_1, \mathcal{K}_2 \in \mathfrak{I}_2$, is a Hilbert space. The above sum converges absolutely and is independent of the orthonormal basis chosen.

Theorem 2.7 (Reed and Simon [60])**.** *Let $X \subseteq \mathbb{R}$. The operator $\mathcal{K} \in \mathbb{B}(\mathbb{H})$ is Hilbert–Schmidt if and only if there is a function $k \in L^2(X\times X)$ with*

$$\mathcal{K}u(x) = \int_X k(x,y)u(y)\mathrm{d}y.$$

Further, we have that

$$\|\mathcal{K}\|_{\mathfrak{I}_2}^2 = \int_X\int_X |k(x,y)|^2\,\mathrm{d}x\mathrm{d}y.$$

[4] An L^2-kernel is Hermitian if $k(x,y) = \overline{k(y,x)}$.

For general Hilbert–Schmidt operators, the sum $\sum_{n=1}^{\infty} \lambda_n^2$ converges absolutely (cf. equation (2.14) or (2.18)). However, the convergence of $\sum_{n=1}^{\infty} \lambda_n$ is not guaranteed, and so the infinite product $\prod_{n=1}^{\infty}(1+\lambda_n)$ might not converge. To resolve this and be able to define a notion of determinant in $\mathfrak{I}_2$, it suffices to consider the infinite product $\prod_{n=1}^{\infty}(1+\lambda_n)\mathrm{e}^{-\lambda_n}$ which is finite. Therefore if $\mathcal{K} \in \mathfrak{I}_2$, the determinant of the operator $(\mathrm{id} + z\mathcal{K})$ is given, for all $z \in \mathbb{C}$, by

$$\prod_{n=1}^{\infty}(1+z\lambda_n)\mathrm{e}^{-z\lambda_n}. \tag{2.15}$$

Remark 2.2.

1. Note that in the expansion of the above infinite product, the value $\sum_{n\geqslant 1} \lambda_n$ vanishes due to opposite signs.

2. In particular, if $\mathcal{K} \in \mathfrak{I}_2$ is an integral operator, the modified Fredholm determinant $d_2(z)$ (2.8) is equal to (2.15), i.e.

$$d_2(z) = \prod_{n=1}^{\infty}(1+z\lambda_n)\mathrm{e}^{-z\lambda_n}.$$

3. If $\mathcal{K} \in \mathfrak{I}_2$ is an integral operator with continuous kernel $k(x,y)$ in $[a,b]\times[a,b]$, then the Fredholm determinant $d(z)$ and the modified Fredholm determinant $d_2(z)$ satisfy (cf. [38, p. 205])

$$d(z) = d_2(z)\exp\bigl(z\int_a^b k(x,x)\mathrm{d}x\bigr).$$

   If $\mathcal{K}$ is of trace class then the above relation holds with $\operatorname{tr}\mathcal{K} = \int_a^b k(x,x)\mathrm{d}x$.

2.3.3 The Schatten–von Neumann class

We have just seen two classes of the Schatten–von Neumann classes of compact operator, namely, trace class and Hilbert–Schmidt operators. Here, we discuss more general classes of compact operators. The Schatten–von Neumann classes of compact operators are defined, for $1 \leqslant p < \infty$, by

$$\mathfrak{I}_p = \{\mathcal{K} \in \mathfrak{I}_\infty \colon \operatorname{tr}|\mathcal{K}|^p < \infty\}.$$

The above space equipped with the norm $\|\mathcal{K}\|_{\mathfrak{I}_p}^p := \mathrm{tr}|\mathcal{K}|^p$ is a Banach space. Moreover, the classes $\mathfrak{I}_p$ are two sided operator ideals in $\mathbb{B}(\mathbb{H})$, i.e. for any $\mathcal{K} \in \mathfrak{I}_p$ and $\mathcal{K}_1, \mathcal{K}_2 \in \mathbb{B}(\mathbb{H})$ we have $\mathcal{K}_1\mathcal{K}\mathcal{K}_2 \in \mathfrak{I}_p$ and

$$\|\mathcal{K}_1\mathcal{K}\mathcal{K}_2\|_{\mathfrak{I}_p} \leqslant \|\mathcal{K}_1\|\|\mathcal{K}\|_{\mathfrak{I}_p}\|\mathcal{K}_2\|, \tag{2.16}$$

where $\|\cdot\|$ is the operator norm defined in (2.9).

Theorem 2.8 (Gohberg et al. [32, Theorem 11.1, Chap IV])**.** *For $p \geqslant 1$, the space $(\mathfrak{I}_p, \|\cdot\|_p)$ is an embedded subalgebra of $\mathbb{B}(\mathbb{H})$ with the approximation property. The algebra $\mathfrak{I}_p$ is complete.*

This implies that for any $\mathcal{K}_1, \mathcal{K}_2 \in \mathfrak{I}_p$, we have (embedded algebra)

$$\|\mathcal{K}_1\| \leqslant \|\mathcal{K}_1\|_{\mathfrak{I}_p} \quad \text{and} \quad \|\mathcal{K}_1\mathcal{K}_2\|_{\mathfrak{I}_p} \leqslant \|\mathcal{K}_1\|_{\mathfrak{I}_p}\|\mathcal{K}_2\|_{\mathfrak{I}_p}.$$

It also implies that the set of finite rank operators is $\|\cdot\|_{\mathfrak{I}_p}$-dense in $\mathfrak{I}_p$ (approximation property).

Theorem 2.9 (Gohberg et al. [32, Theorem 11.2, Chap IV])**.** *Let $p, p_1, \ldots, p_n$ be some positive numbers such that*

$$\frac{1}{p} \leqslant \frac{1}{p_1} + \frac{1}{p_2} + \cdots + \frac{1}{p_n}.$$

If $\mathcal{K}_j \in \mathfrak{I}_{p_j}$ $(j = 1, 2, \ldots, n)$, then the operator $\mathcal{K} = \mathcal{K}_1\mathcal{K}_2 \cdots \mathcal{K}_n \in \mathfrak{I}_p$ and

$$\|\mathcal{K}\|_{\mathfrak{I}_p} \leqslant \prod_{j=1}^{n} \|\mathcal{K}_j\|_{\mathfrak{I}_{p_j}}.$$

Clearly from the above theorem, we have if $\mathcal{K} = \mathcal{K}_1\mathcal{K}_2$ with $\mathcal{K}_1, \mathcal{K}_2 \in \mathfrak{I}_2$ that

$$\|\mathcal{K}\|_{\mathfrak{I}_1} \leqslant \|\mathcal{K}_1\|_{\mathfrak{I}_2}\|\mathcal{K}\|_{\mathfrak{I}_2}.$$

Moreover, for any $p \leqslant q$, the following inequality holds (the continuous embeddings):

$$\|\mathcal{K}\|_{\mathfrak{I}_q} \leqslant \|\mathcal{K}\|_{\mathfrak{I}_p}. \tag{2.17}$$

By Weyl's inequality, we have

$$|\operatorname{tr} \mathcal{K}^p| \leqslant \|\mathcal{K}^p\|_{\mathfrak{I}_p} \leqslant \|\mathcal{K}\|_{\mathfrak{I}_p}^p. \tag{2.18}$$

2.4 Modified/regularised Fredholm determinants

Let $\mathcal{K} \in \mathfrak{I}_p$ with eigenvalues $\{\lambda_n\}_{n\geqslant 1}$. Then for all $z \in \mathbb{C}$ and $p \in \mathbb{N} \setminus \{0\}$, the Plemelj–Smithies formula for p-modified Fredholm determinants is given by (cf. [32] and [67])

$$\det_p(\mathrm{id} + z\mathcal{K}) = \sum_{n=0}^{\infty} z^n \alpha_n^{(p)}/n!, \tag{2.19}$$

where $\alpha_0^{(p)} = 1$, and

$$\alpha_n^{(p)} = \det_{\mathbb{C}^n} \begin{pmatrix} \nu_1^{(p)} & n-1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \nu_{n-1}^{(p)} & \nu_{n-2}^{(p)} & \cdots & \cdots & 1 \\ \nu_n^{(p)} & \nu_{n-1}^{(p)} & \cdots & \cdots & \nu_1^{(p)} \end{pmatrix} \tag{2.20}$$

with

$$\nu_j^{(p)} = \begin{cases} \operatorname{tr} \mathcal{K}^j, & j \geqslant p \\ 0, & j \leqslant p-1. \end{cases} \tag{2.21}$$

For all natural numbers $p \geqslant 1$, the coefficients $\alpha_n^{(p)}$ satisfy (Simon [67])

$$\alpha_n^{(p)} = \sum_{j=1}^{n} (-1)^{j+1} \alpha_{n-j}^{(p)} \nu_j^{(p)} \frac{(n-1)!}{(n-j)!}. \tag{2.22}$$

Equivalently, p-modified Fredholm determinants can be expressed as follows:

1. For all $z \in \mathbb{C}$ (cf. [65], [32] and [67]),

$$\det_p(\mathrm{id} + z\mathcal{K}) = \prod_{n=1}^{\infty} \Big[(1 + z\lambda_n) \exp\Big(\sum_{j=1}^{p-1} z^j (-\lambda_n)^j / j \Big) \Big]; \tag{2.23}$$

2. For small $z \in \mathbb{C}$, Plemelj's formula is given by (cf. [65], [32] and [67])

$$\det_p(\mathrm{id} + z\mathcal{K}) = \exp\Big(\sum_{n=p}^{\infty}(-1)^{n+1} z^n \mathrm{tr}\, \mathcal{K}^n/n\Big) \tag{2.24}$$

which can be analytically continued as an entire function to all $z \in \mathbb{C}$;

We have for any $\mathcal{K} \in \mathfrak{I}_{p-1}$ $(p \geqslant 2)$ that (cf. [65], [32] and [67])

$$\det_p(\mathrm{id} + z\mathcal{K}) = \det_{p-1}(\mathrm{id} + z\mathcal{K}) \exp\left((-z)^{p-1} \mathrm{tr}\, \mathcal{K}^{p-1}/(p-1)\right). \tag{2.25}$$

Theorem 2.10 (Gohberg et al. [32])**.** *Let $\mathcal{K} \in \mathfrak{I}_p$. Then, the operator $(\mathrm{id} + \mathcal{K})$ is invertible if and only if $\det_p(\mathrm{id} + \mathcal{K}) \neq 0$.*

Theorem 2.11 (Gohberg et al. [32])**.** *If $z = -\lambda_0^{-1}$ is a zero with a given order of the entire function $\det_p(\mathrm{id} + z\mathcal{K})$ then λ_0 is an eigenvalue of the operator $\mathcal{K} \in \mathfrak{I}_p$ with the exact same algebraic multiplicity.*

We have collected some inequalities, theorems and properties we use in this thesis. For other results on infinite determinants, see for example [67] and [32]. The next chapter concerns the Evans function and its properties.

Remark 2.3. Throughout this thesis, the trace 'tr' is associated with bounded operators in Hilbert space, and '$\mathrm{tr}_{\mathbb{F}^n}$' will refer to the trace of any square matrix over the field $\mathbb{F}$. The determinant of a square matrix will be denoted by $\det_{\mathbb{F}^n}$, for $n \in \mathbb{N}$.

Chapter 3

The Evans function

This chapter presents the formulation of the concerned eigenvalue problems, and also some constructions of the Evans function. We consider eigenvalue problems arising from linearising a nonlinear partial differential equation about its stationary solution. Thus, the stability analysis of the stationary solution reduces to computing eigenvalues of the linear differential operator associated with the problem. Although there are many methods for computing these eigenvalues, in this thesis we focus on the Evans function and the Fredholm determinant (see previous chapter). The Evans function, first introduced in [23] and then generalised in [1], is an analytic function of the spectral parameter whose zeros of a given order coincide in location and in algebraic multiplicity to eigenvalues of the corresponding linear differential operator. The Evans function is a major tool used in the stability analysis of travelling waves (see, e.g. [9], [14], [26], [40], [45], and [52]).

3.1 Set up for the eigenvalue problem

Consider a system of nonlinear partial differential equations (PDEs) given by

$$\partial_t U = \mathcal{L}_0 U + \mathcal{N}(U), \tag{3.1}$$

where as a function of $x \in \mathbb{R}$, $U(\cdot, t) \in \mathbb{C}^n$ $(n \geqslant 1)$ is in some appropriate Banach space, $\mathcal{L}_0$ denote a closed, densely defined linear differential operator with respect to the space variable x, $\mathcal{N}$ denotes the nonlinearity defined not necessarily on the entire space associated with U, t is the time variable.

Changing the coordinates (x,t) to a moving frame $(x \to x - ct, t)$, equation (3.1) becomes

$$\partial_t U = \mathcal{L}_0 U + c\partial_x U + \mathcal{N}(U). \tag{3.2}$$

Definition 3.1. A travelling wave ϕ of (3.2) is a solution of the form

$$U(x,t) = \phi(x - ct)$$

corresponding to a fixed profile ϕ that travels to the right ($c > 0$) or to the left ($c < 0$) as a function of time $t \in \mathbb{R}^+$, where $x \in \mathbb{R}$ is the space coordinate and c is the wave speed.

If it exists, the travelling wave ϕ satisfies the following equation

$$\mathcal{L}_0\phi + c\partial_x\phi + \mathcal{N}(\phi) = 0. \tag{3.3}$$

In this thesis, we will only consider travelling waves with finite limits at infinity, i.e.

$$\lim_{x\to\pm\infty} \phi(x) = \phi^{\pm} \in \mathbb{R}^n. \tag{3.4}$$

A travelling wave ϕ is a *pulse* if $\phi^- = \phi^+$, otherwise it is a *front*. In turns, these correspond to homoclinic and heteroclinic orbits associated with homogeneous fixed points of problem (3.3) respectively. Assuming the existence and the uniqueness of the travelling wave ϕ, the goal is to determine its stability, in particular linear stability. Note that, if $\phi(x)$ is a travelling wave then so is $\phi(x + \nu)$, for any $\nu \in \mathbb{R}$.

Definition 3.2. [1, p. 170] A travelling wave ϕ is said to be asymptotically stable relative to (3.2), if there is a neighborhood N of ϕ in some appropriate Banach space so that for a given initial condition $U_0 \in N$ and U a solution of problem (3.2), then there is a ν for which

$$\|U(\cdot,t) - \phi(\cdot + \nu)\| \to 0, \quad \text{as} \quad t \to \infty.$$

$\|\cdot\|$ is the norm in an appropriate Banach space.

As in the stability analysis of autonomous dynamical systems, the problem in the

moving frame (3.2) is linearised about the travelling wave ϕ, with perturbation u off ϕ given, for $\lambda \in \mathbb{C}$, by

$$u(x,t) = u(x)\mathrm{e}^{\lambda t}.$$

Upon neglecting the nonlinear terms in u, and using the equation for the travelling wave (3.3), this yields

$$\lambda u = \mathcal{L}_0 u + c\partial_x u + \partial_\phi \mathcal{N}(\phi)u. \tag{3.5}$$

Setting

$$\mathcal{L} \coloneqq \mathcal{L}_0 + c\partial_x + \partial_\phi \mathcal{N}(\phi), \tag{3.6}$$

the stability of the travelling wave ϕ reduces to computing eigenvalues associated with the closed, densely defined operator $\mathcal{L}$. Note that the spectrum of operator $\mathcal{L}$ is non-empty, since $\lambda = 0$ is an eigenvalue associated with translational invariance. In fact, if the differential operator $\mathcal{L}_0$ has constant coefficients then $\mathrm{d}\phi/\mathrm{d}x$ is the corresponding eigenfunction. Indeed, substituting $\mathrm{d}\phi/\mathrm{d}x$ in the eigenvalue problem (3.5) and using (3.3), we see that

$$\mathcal{L}_0 \frac{\mathrm{d}}{\mathrm{d}x}\phi + c\partial_x \frac{\mathrm{d}}{\mathrm{d}x}\phi + \partial_\phi \mathcal{N}(\phi)\frac{\mathrm{d}}{\mathrm{d}x}\phi = \frac{\mathrm{d}}{\mathrm{d}x}\big(\mathcal{L}_0\phi + c\partial_x\phi + \mathcal{N}(\phi)\big) = 0.$$

3.2 The Evans functions

A convenient way to deal with the eigenvalue problem (3.5) is to rewrite it as a first order linear system of differential equations (ODEs)

$$\frac{\mathrm{d}}{\mathrm{d}x}Y = A(x,\lambda)Y, \tag{3.7}$$

where $A(x,\lambda)$ is analytic in $\lambda \in \mathbb{C}$ and $Y \in \mathbb{C}^{2n}$. Note that due to the asymptotic limits of the travelling wave ϕ in (3.4), the matrix-valued function $A(x,\lambda)$ has finite far field limits:

$$\lim_{x\to\pm\infty} A(x,\lambda) = A^{\pm}(\lambda). \tag{3.8}$$

The *essential spectrum* $\sigma_e(\mathcal{L})$ of a closed, densely defined operator $\mathcal{L}$ is defined as the complement of the pure point specturm in $\sigma(\mathcal{L})$. Throughout this thesis, $\Lambda \subseteq (\mathbb{C} \setminus \sigma_e(\mathcal{L}))$ is an open connected subregion of the λ-complex plane to the right

of $\sigma_e(\mathcal{L})$. If $\sigma_e(\mathcal{L})$ impinges onto the right-half plane, we can always invoke weight functions to push $\sigma_e(\mathcal{L})$ into the left-half plane.

Let $\lambda \in \Lambda$. For $j = 1, \ldots, r$, let $\kappa_j^-(\lambda)$, denote eigenvalues of $A^-(\lambda)$ with positive real parts, and for $j = r+1, \ldots, 2n$, let $\kappa_j^+(\lambda)$ denote eigenvalues of $A^+(\lambda)$ with negative real parts. For all $\lambda \in \Lambda$, we assume that $\kappa_j^\pm = \kappa_j^\pm(\lambda)$ are simple and that

$$\|A(\cdot, \lambda) - A^\pm(\lambda)\|_{\mathbb{C}^{2n\times 2n}} \in L^1(\mathbb{R}, \mathbb{C}). \tag{3.9}$$

Then there exists a r-dimensional unstable subspace E^- and $(2n-r)$-dimensional stable subspace E^+ defined by

$$E^\pm = \{Y_j^\pm \in \mathbb{C}^{2n} \colon \lim_{x\to\pm\infty} Y_j^\pm(x,\lambda)\mathrm{e}^{-\kappa_j^\pm x} = \eta_j^\pm(\lambda)\},$$

where $Y_j^\pm$ satisfy the first order system (3.7) and $\eta_j^\pm(\lambda)$ are the eigenvectors associated with the eigenvalues $\kappa_j^\mp$. The first order systems (3.7) admits a square integrable solution on the real line for a given $\lambda \in \mathbb{C}$ (i.e. λ is an eigenvalue of the operator $\mathcal{L}$) if and only if the subspaces $E^\pm$ have nontrivial intersection. In other words, λ is an eigenvalue if and only if the spanning vectors of the subspaces $E^\pm$ are collectively linearly dependent. The Evans function $E(\lambda)$ as introduced in [23] enables us to measure this linear dependence, and it is given by

$$E(\lambda) = \exp\Big(-\int_0^x \mathrm{tr}_{\mathbb{C}^{2n}} A(s,\lambda)\mathrm{d}s\Big)\det{}_{\mathbb{C}^{2n}}\begin{pmatrix} Y_1^- & \cdots & Y_k^- & Y_{2n-r}^+ & \cdots & Y_{2n}^+ \end{pmatrix}. \tag{3.10}$$

Note that the Evans function $E(\lambda)$ is independent of the variable x. The following construction, due to Swinton [69], assumes that either κ_j^+ or κ_j^- are simple, since it relies on the formal adjoint problem of (3.7), i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}x}Z = -\big(A(x,\lambda)\big)^* Z, \tag{3.11}$$

where A^* is the conjugate transpose of A, and $Z \in \mathbb{C}^{2n}$. For all $Y_j, Z_i \in \mathbb{C}^{2n}$ satisfying (3.7) and (3.11) respectively, the following equation holds

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}(Z_i^* Y_j) &= -(A(x,\lambda)^* Z_i)^* Y_j + Z_i^* A(x,\lambda) Y_j \\ &= -Z_i^* A(x,\lambda) Y_j + Z_i^* A(x,\lambda) Y_j \\ &= 0.\end{aligned}$$

This implies that the product $Z_i^* Y_j$ is constant as a function of x and depends only on the spectral parameter λ. In other words, the vectors Z_i are orthogonal to Y_j. Let $Z^{\pm}$ denote the solutions of the adjoint problem (3.11) that decay at $\pm\infty$, and $E_*^{\pm}$ the subspaces spanned by these solutions respectively. Note that since $\big((Z_i^{\pm})^* Y_j^{\pm}\big)(\pm\infty, \lambda) = 0$, the subspaces $E_*^{\pm}$ are orthogonal to the subspaces $E^{\pm}$ respectively. Hence for a given $\lambda \in \Lambda$, if the subspaces $E^{\pm}$ are orthogonal to the subspaces $E_*^{\mp}$, then the subspaces $E^{\pm}$ have a nontrivial intersection.
The orthogonality condition of the subspaces $E^{\pm}$ and $E_*^{\mp}$ is measured by an analytic function $E_S(\lambda)$ which is defined, for example, by

$$E_S(\lambda) = \det_{\mathbb{C}^r} \begin{pmatrix} \langle Z_1^-, Y_1^+ \rangle_{\mathbb{C}^n} & \cdots & \langle Z_1^-, Y_r^+ \rangle_{\mathbb{C}^n} \\ \vdots & \ddots & \vdots \\ \langle Z_r^-, Y_1^+ \rangle_{\mathbb{C}^n} & \cdots & \langle Z_r^-, Y_r^+ \rangle_{\mathbb{C}^n} \end{pmatrix}, \tag{3.12}$$

where $\langle Z_i, Y_j \rangle_{\mathbb{C}^n} = \sum_{l=1}^{2n} \overline{Z}_{il} Y_{jl}$, where Y_{jl} is the lth component of Y_j. The zeros of the Evans function $E_S(\lambda)$ coincide with eigenvalues of $\mathcal{L}$. The simplicity assumption of eigenvalues $\kappa_j^{\pm}$ is not needed in the construction of the Evans function of Alexander et al. [1]. This construction is based on expressing equation (3.7) in the exterior algebra framework (see Appendix A). Consequently, the stable and unstable subspaces are associated with a single exponential decay and growth mode respectively. The Evans function of Alexander et al. is given by

$$E_A(\lambda) = \exp\left(-\int_0^x \mathrm{tr}_{\mathbb{C}^{2n}} A(s,\lambda)\mathrm{d}s \right) Y^-(x,\lambda) \wedge Y^+(x,\lambda), \tag{3.13}$$

where $Y^+ \in \bigwedge^{2n-r} \mathbb{C}^{2n}$ and $Y^- \in \bigwedge^{r} \mathbb{C}^{2n}$ satisfy

$$\frac{\mathrm{d}}{\mathrm{d}x} Y^+ = A^{(2n-r)}(x,\lambda) Y^+ \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}x} Y^- = A^{(r)}(x,\lambda) Y^- \tag{3.14}$$

respectively. The matrices $A^{(r)}$ and $A^{(2n-r)}$ are those on $\bigwedge^{r} \mathbb{C}^{2n}$ and $\bigwedge^{n-r} \mathbb{C}^{2n}$ induced by A, respectively. The forms Y^+ and Y^- satisfy the asymptotic estimates

$$\lim_{x \to \pm\infty} \mathrm{e}^{-\tilde{\kappa}^{\pm} x} Y^{\pm}(x,\lambda) = \widetilde{\eta}^{\pm}(\lambda),$$

where $\tilde{\kappa}^+$ and $\tilde{\kappa}^-$ are the eigenvalues of $A_+^{(2n-r)}(\lambda)$ and $A_-^{(r)}(\lambda)$ with negative and positive real parts respectively, and $\widetilde{\eta}^{\mp}(\lambda)$ are the corresponding eigenvectors. The Evans function of Alexander et al. $E_A(\lambda)$ satisfies (see Bridges and Derks [12] and [13])

$$\begin{aligned} E_A(\lambda) &\equiv [\![\star \widetilde{Y}^-, Y^+]\!]_{2n-r} \\ &= C(\lambda) [\![Z^-, Y^+]\!]_{2n-r}, \end{aligned}$$

where $\widetilde{Y}^- = \mathrm{e}^{-\int_0^x \mathrm{tr}_{\mathbb{C}^{2n}} A(s,\lambda)\mathrm{d}s} Y^-$, $Z^- \in \bigwedge^{2n-r} \mathbb{C}^{2n}$ satisfies the adjoint problem of the first equation in (3.14), $C(\lambda)$ is a nonvanishing analytic function, $[\![\cdot, \cdot]\!]_{2n-r}$ is the inner product on $\bigwedge^{2n-r} \mathbb{C}^{2n}$ and $\star$ denotes the Hodge star operator (see Appendix A). Note that if either κ_j^- or κ_j^+ are simple then $[\![Z^-, Y^+]\!]_{2n-r} = E_S(\lambda)$, since the $(2n-r)$-forms Z^- and Y^+ can be recovered with $(2n-r)$-analytic basis vector solutions of problems (3.11) and (3.7), respectively. When $\kappa_j^{\pm}$ are not simple, Bridges and Derks [13] have shown that one can still construct analytic basis vectors associated with the forms Y^+ and Z^-. Hence an equality similar to that between $E_S(\lambda)$ and the inner product of Z^- and Y^+ on $\bigwedge^{2n-r} \mathbb{C}^{2n}$ holds. Furthermore, Kapitula and Sandstede [45] have shown how to analytically extend the Evans function $E_A(\lambda)$ to some points λ where $A^{\pm}(\lambda)$ fails to be hyperbolic. All the Evans functions are equal up to a nonvanishing analytic function. Hence for any Evans function, we have the following.

Theorem 3.1. *[64] The Evans function $E(\lambda)$ in (3.10) is analytic in $\lambda \in \Lambda$ with the following properties:*

1. *The value of the Evans function $E(\lambda)$ at $\lambda = 0$ is 0.*

2. *The Evans function $E(\lambda)$ is real whenever $\lambda \in \Lambda$ is real.*

3. *$E(\lambda) = 0$ if and only if λ is an eigenvalue of $\mathcal{L}$.*

4. *The order of any zero of the Evans function $E(\lambda)$ is equal to the algebraic multiplicity of the corresponding eigenvalue.*

Chapter 4

Fredholm determinants and the Evans function

This chapter establishes the connection between the Fredholm determinant and the Evans function. This in turns yields a reduction to a finite dimensional determinant, the determinant of the differential operator associated with the eigenvalue problem. The connection found in Gesztesy et al. [27] is based on the semi-separability property of the kernel function, whereas in this chapter a finite dimensional determinant which measures the intersection of the subspaces decaying at plus/minus infinity is constructed. That is, if the subspaces decaying at plus/minus infinity of the perturbed and unperturbed adjoint problems are orthogonal, then the subspaces decaying at plus/minus infinity of the perturbed problem intersect (i.e. an eigenvalue is detected). This is because the subspaces decaying at plus/minus infinity associated with the unperturbed and its adjoint problems are orthogonal. Thus, measuring the orthogonality is equivalent to computing a determinant similar to that given in (3.12) which is evaluated at infinity. By analogy to the transmission coefficient in Scattering Theory, the matrix associated with the finite dimensional determinant is called the *matrix transmission coefficient*. The basic details reducing the Fredholm determinant to the Evans function are as follows.

1. Proving that the determinant of the matrix transmission coefficient is equal to the Fredholm determinant associated with the underlying trace class integral operator;

2. Showing that the determinant of the matrix transmission coefficient is equal to

the Evans function, up to a nonvanishing analytic function. Combining this relation with that of item 1, the connection between the Evans function and the Fredholm determinant follows;

3. Given both the connections in item 2 and 1, the reduction of item 2 is extended to any operator in the Schatten–von Neumann class;

4. Exploiting the multiplicative property of the determinant for an unbounded elliptic operator and a trace class perturbation of the identity operator, the determinant of the differential operator associated with the eigenvalue problem reduces to the Evans function, up to a non-vanishing analytic function.

4.1 The integral reformulation

In this section, we reformulate the first order systems given in (3.7) of the travelling wave problem of Chapter 3 into an integral problem. We then analyse the properties of the corresponding integral operator. We also identify a class of eigenvalue problems for which the associated integral operator is of trace class.

Theorem 4.1 (Green's function, [49])**.** *Let $\mathcal{L}$ be an nth order ordinary differential operator with bounded and continuous coefficients $a_j = a_j(x),\ j = 0, \ldots, n$. Then the Green's function $g(x, y)$ satisfies*

$$\mathcal{L}g(x, y) = \delta(x - y)$$

in the sense of distributions if and only if :

1. *$g(x, y)$ is $(n - 2)$ times continuously differentiable in x at $x = y$;*
2. *$\left[\partial_x^{n-1} g(x, y)\right]_{x=y^-}^{x=y^+} = \frac{1}{a_n}$ (jump condition).*
3. *The Green's function $g(x, y)$ satisfies the appropriate boundary conditions in the x-variable.*

If $\mathcal{K}$ denotes the right inverse of $\mathcal{L}$, then the solution of $\mathcal{L}u = f$ is given by

$$u(x) = \mathcal{K}f(x) = \int_{\mathbb{R}} g(x, y) f(y) \mathrm{d}y.$$

The Green's function of a closed ordinary differential operator in any interval, in particular on the real line, is *semi-separable*. This means that,

$$g(x,y) = \begin{cases} F_1(x)G_1(y), & y \leqslant x, \\ F_2(x)G_2(y), & x < y, \end{cases} \tag{4.1}$$

where $F_j \in L^2(\mathbb{R}, \mathbb{C}^{n\times n_j})$ and $G_j \in L^2(\mathbb{R}, \mathbb{C}^{n_j \times n})$ for $j = 1, 2$ and $1 \leqslant n_j \leqslant n$.

Definition 4.1 (Fredholm operator, [31])**.** A bounded operator $\mathcal{K}$ acting between Banach spaces (normed spaces) E and F is *Fredholm* if its range $\mathrm{ran}(\mathcal{K})$ is closed and the numbers

$$n(\mathcal{K}) = \dim(\mathrm{Ker}(\mathcal{K})) \quad \text{and} \quad d(\mathcal{K}) = \dim(F/\mathrm{ran}(\mathcal{K})) \tag{4.2}$$

are finite. The *index* of $\mathcal{K}$ is given by $\mathrm{ind}(\mathcal{K}) = n(\mathcal{K}) - d(\mathcal{K})$.

For any compact operator $\mathcal{K}$, the operator $\mathrm{id}+\mathcal{K}$ is Fredholm of index zero (cf. [31]). In what follows, we shall denote by $\det_F(\mathcal{A})$ the determinant of any Fredholm operator $\mathcal{A}$ (cf. Section 4.4 for the well definedness of the determinant). If $\mathcal{A} = \mathrm{id} + \mathcal{K}$ with $\mathcal{K} \in \mathfrak{I}_p$, we write

$$\det_F(\mathcal{A}) \coloneqq \det_p(\mathrm{id} + \mathcal{K}).$$

Throughout this thesis, for $n \in \mathbb{N}$, H^n will denote the Sobolev space of functions with derivative up to order n in L^2 on $\mathbb{R}$.

4.1.1 The integral operator and its properties

Consider the following eigenvalue problem

$$\mathcal{T}(\lambda)Y = 0, \tag{4.3}$$

where $Y \in \mathbb{C}^{2n}$ with $n \geqslant 1$, and

$$\mathcal{T}(\lambda) \coloneqq \mathrm{d}/\mathrm{d}x - A(\cdot, \lambda) \tag{4.4}$$

is a closed, densely defined operator for λ in some suitable region of $\mathbb{C}$. Assume that $A\colon \mathbb{R}\times\mathbb{C}\to\mathbb{C}^{2n\times 2n}$ is analytic in $\lambda\in\mathbb{C}$ and decomposes into

$$A(\cdot,\lambda) = A_0(\cdot,\lambda) + V(\cdot), \tag{4.5}$$

where the bounded and continuous operator $A_0(x,\cdot)$ represents the unperturbed part of $A(x,\cdot)$, and the perturbation V satisfies

$$\|V\|_{\mathbb{C}^{2n\times 2n}} \in L^1(\mathbb{R},\mathbb{C})\cap L^\infty(\mathbb{R},\mathbb{C}). \tag{4.6}$$

Our objective is to determine the values of $\lambda\in\mathbb{C}$ for which $\dim\operatorname{Ker}\mathcal{T}(\lambda)>0$, where

$$\mathcal{T}(\lambda)\colon H^1(\mathbb{R},\mathbb{C}^{2n})\to L^2(\mathbb{R},\mathbb{C}^{2n})$$

In other words, we seek $\lambda\in\mathbb{C}$ such that the eigenvalue problem (4.3) has nontrivial solutions in the L^2 sense.

Remark 4.1. Assume that the perturbation V satisfies $\lim_{|x|\to\infty}V(x)=V_0$, where V_0 is nonzero matrix. If $\|V-V_0\|_{\mathbb{C}^{2n\times 2n}}\in L^1(\mathbb{R},\mathbb{C})$, then the same analysis holds with $V-V_0$ and $A_0(\cdot,\lambda)+V_0$ substituted for V and $A_0(\cdot,\lambda)$ respectively.

Remark 4.2. For travelling wave problems, the following statements are valid:

1. The nonzero entries in the perturbation matrix V depend on the travelling wave ϕ;

2. We have $\lambda=0$ is an eigenvalue due to the translational invariance (cf. Chapter 3).

In what follows, we assume the non-emptiness of the resolvent set ρ associated with the operator

$$\mathcal{T}_0(\lambda) \coloneqq \mathrm{d}/\mathrm{d}x - A_0(\cdot,\lambda), \tag{4.7}$$

and we denote by $\mathcal{K}_0(\lambda)$ the corresponding resolvent operator. Then given the decomposition of the matrix A in (4.5), we write

$$\mathcal{T}(\lambda) = \mathcal{T}_0(\lambda)\big(\mathrm{id}-\mathcal{K}_0(\lambda)V\big). \tag{4.8}$$

Consequently, if $\mathcal{T}_0(\lambda)$ is invertible then the invertibility of $\mathcal{T}(\lambda)$ depends on that of

$\big(\mathrm{id} - \mathcal{K}_0(\lambda)V\big)$. Therefore, if the operator $\mathcal{K}_0(\lambda)V$, which is analytic in $\lambda \in \rho$ (cf. [31] and [60]) is compact, then λ is an eigenvalue of the operator $\mathcal{T}(\cdot)$ if and only if

$$\det_F\big(\mathrm{id} - \mathcal{K}_0(\lambda)V\big) = 0. \tag{4.9}$$

Indeed, using the decomposition of A in (4.5), the first order system (4.3) becomes, for all $\lambda \in \mathbb{C}$,

$$\mathcal{T}_0(\lambda)Y = VY. \tag{4.10}$$

For now suppose that $\mathcal{T}_0(\lambda)$ is invertible (this shall be proved later). Then, for all $\lambda \in \rho$, we have

$$\big(\mathrm{id} - \mathcal{K}_0(\lambda)V\big)Y = 0. \tag{4.11}$$

That is, the eigenvalue problem (4.3) is reduced to an integral eigenvalue problem given as above. Note that equation (4.8) assumes the existence of the right inverse which follows from the existence of the Green's function (cf. Theorem 4.1). To obtain equation (4.11) from equation (4.10), we moreover assume the existence of the left inverse. Therefore by invertibility we mean the existence of the left and the right inverse, i.e.,

$$\mathcal{K}\mathcal{L} = \mathcal{L}\mathcal{K} = \mathrm{id}, \tag{4.12}$$

where $\mathcal{L}$ is an operator in some Banach space and $\mathcal{K}$ its inverse.

Given the resolvent operator $\mathcal{K}_0(\lambda)$, there exists an exponential dichotomy on $\mathbb{R}$ (see [64, Theorem 3.2]) of the following equation

$$\mathcal{T}_0(\lambda)Y = 0. \tag{4.13}$$

We recall that for fixed $\lambda \in \rho$, equation (4.13) has an exponential dichotomy on $\mathbb{R}$, if for some positive constants κ', κ and c, the following inequalities hold for all $x, y \in \mathbb{R}$

$$\begin{aligned} \|\Phi(x,\lambda)Q\Phi^{-1}(y,\lambda)\|_{\mathbb{C}^{2n\times 2n}} &\leqslant c(\kappa')\mathrm{e}^{-\kappa'(y-x)}, \quad x \leqslant y \\ \|\Phi(x,\lambda)(\mathrm{id}_{2n} - Q)\Phi^{-1}(y,\lambda)\|_{\mathbb{C}^{2n\times 2n}} &\leqslant c(\kappa)\mathrm{e}^{-\kappa(x-y)}, \quad x \geqslant y, \end{aligned} \tag{4.14}$$

where Q is the projection operator onto the subspace decaying at $-\infty$ associated with

problem (4.13), and $\Phi(\cdot,\lambda)$ is a fundamental matrix which is chosen to be analytic in $\lambda \in \rho$. $\Phi(\cdot,\lambda)$ is a fundamental matrix solution if its column vectors are $2n$ linearly independent solutions of (4.13), i.e. $\mathcal{T}_0(\lambda)\Phi(x,\lambda) = 0$. Since $\rho \neq \emptyset$, the operator $\mathcal{T}_0(\lambda)$ is closed (cf. [31, Chap XIV]). Hence the Green's function k_0 associated with the operator $\mathcal{T}_0(\lambda)$ is of the form given by (4.1), i.e.

$$k_0(x,y;\lambda) = \begin{cases} -\Phi(x,\lambda)Q\Phi^{-1}(y,\lambda), & x \leqslant y \\ \Phi(x,\lambda)(\mathrm{id}_{2n} - Q)\Phi^{-1}(y,\lambda), & x > y. \end{cases} \tag{4.15}$$

The resolvent operator $\mathcal{K}_0(\lambda)$ with the above kernel is invertible, i.e. it satisfies the invertibility equations (4.12). Indeed from Theorem 4.1, it follows that

$$\mathcal{T}_0(\lambda)\big(\mathcal{K}_0(\lambda)Y\big) = Y$$

and by integration by parts we have

$$\begin{aligned} \mathcal{K}_0(\lambda)\big(\mathcal{T}_0(\lambda)Y(x)\big) &= \int_{\mathbb{R}} k_0(x,y;\lambda)\mathcal{T}_0(\lambda)Y(y)\mathrm{d}y \\ &= k_0(x,y;\lambda)Y(y)\Big|_{y=-\infty}^{y=+\infty} - \int_{\mathbb{R}} \mathcal{T}_0^*(\lambda)k_0(x,y;\lambda)Y(y)\mathrm{d}y \\ &= Y(x) \end{aligned}$$

where $\mathcal{T}_0^*(\lambda)$ is the formal adjoint of $\mathcal{T}_0(\lambda)$, and $Y(x) \coloneqq Y(x,\lambda)$. Assume for the moment that $\mathcal{K}_0(\lambda)V$ is compact. Then invoking the Fredholm alternative, we have that either 1 is an eigenvalue of $\mathcal{K}_0(\lambda)V$ or $\det_F\big(\mathrm{id} - \mathcal{K}_0(\lambda)V\big)$ is nonzero. Consequently, if 1 is an eigenvalue of $\mathcal{K}_0(\lambda)V$, then λ is eigenvalue of $\mathcal{T}(\cdot)$. However, it is not clear that the order of the zeros of $\det_F\big(\mathrm{id} - \mathcal{K}_0(\lambda)V\big)$ and the algebraic multiplicities of eigenvalues of $\mathcal{T}(\cdot)$ coincide.

By rewriting the operator $\mathcal{K}_0(\lambda)V$ in an appropriate form, the multiplicity issue is resolved by the *Birman–Schwinger principle*. To this end, let $V = U|V|$ be the polar decomposition, where U is a partial isometry, and $\Psi = U|Y|^{1/2}$. Then for all

$\Psi \in L^2(\mathbb{R}, \mathbb{C}^{2n})$ and $\lambda \in \rho$, the integral equation (4.11) becomes,

$$\big(\mathrm{id} - \mathcal{K}(\lambda)\big)\Psi = 0, \tag{4.16}$$

where

$$\mathcal{K}(\lambda) = |V|^{1/2}\mathcal{K}_0(\lambda)\widetilde{V} \tag{4.17}$$

is the *Birman–Schwinger operator* with $\widetilde{V} = U|V|^{1/2}$. The Birman–Schwinger principle states that 1 is an eigenvalue of $\mathcal{K}(\lambda)$, if and only if, λ is an eigenvalue of $\mathcal{T}(\cdot)$ with the same algebraic multiplicity (defined as the order of the zero of $\det_F \mathcal{T}(\lambda)$) (cf. [28] and [66]). For all $\lambda \in \rho$, the kernel associated with the operator $\mathcal{K}(\lambda)$ is

$$k(x, y; \lambda) = |V(x)|^{1/2} k_0(x, y; \lambda)\widetilde{V}(y). \tag{4.18}$$

Given the exponential dichotomy inequalities in (4.14), there exists a positive constant $\tilde{\kappa} \leqslant \min\{\kappa', \kappa\}$ and $c(\tilde{\kappa}) > 0$ such that, for fixed $\lambda \in \rho$ and for all $x, y \in \mathbb{R}$,

$$\|k(x, y; \lambda)\|_{\mathbb{C}^{2n\times 2n}} \leqslant c(\tilde{\kappa})\|V(x)\|^{1/2}_{\mathbb{C}^{2n\times 2n}} \mathrm{e}^{-\tilde{\kappa}|x-y|}\|V(y)\|^{1/2}_{\mathbb{C}^{2n\times 2n}}. \tag{4.19}$$

The above estimate follows from using the inequalities

$$\|\widetilde{V}\|_{\mathbb{C}^{2n\times 2n}} \leqslant \|V\|^{1/2}_{\mathbb{C}^{2n\times 2n}} \quad \text{and} \quad \||V|^{1/2}\|_{\mathbb{C}^{2n\times 2n}} \leqslant \|V\|^{1/2}_{\mathbb{C}^{2n\times 2n}}. \tag{4.20}$$

Since $\mathrm{e}^{-\tilde{\kappa}|x-y|}$ is bounded (say by $M > 0$ up to $c(\tilde{\kappa})$) and continuous in $\mathbb{R} \times \mathbb{R}$, it follows that

$$\begin{aligned}\iint \|k(x, y; \lambda)\|^2_{\mathbb{C}^{2n\times 2n}} \mathrm{d}x\mathrm{d}y &\leqslant M^2 \iint \|V(x)\|_{\mathbb{C}^{2n\times 2n}}\|V(y)\|_{\mathbb{C}^{2n\times 2n}} \mathrm{d}x\mathrm{d}y \\ &= M^2\Big(\int_{\mathbb{R}} \|V(x)\|_{\mathbb{C}^{2n\times 2n}} \mathrm{d}x\Big)^2. \end{aligned} \tag{4.21}$$

Consequently, the right-hand side of (4.19) is in $L^2(\mathbb{R}^2, \mathbb{C})$. Hence, the integral operator $\mathcal{K}(\lambda)$ is of Hilbert–Schmidt class in $L^2(\mathbb{R}, \mathbb{C}^{2n})$. However in the next theorem, we show for some classes of operator $\mathcal{T}_0(\lambda)$ that the compact operator $\mathcal{K}(\lambda)$ is, in fact, a trace class operator. First, we recall the following proposition.

Proposition 4.1 (Simon [66])**.** *Let $f = f(x), h = h(x)$ denote the maximally defined*

multiplication operators by f, h, respectively, and $g = g(p)$ the maximal multiplication operator by g in the Fourier space. If $f, h \in L^2$ and $g \in L^1$ then fgh is a trace class operator and

$$\|fgh\|_{\mathfrak{I}_1} \leqslant (2\pi)^{-1}\|f\|_{L^2}\|h\|_{L^2}\|g\|_{L^1}. \tag{4.22}$$

We now present one of our main results.

Theorem 4.2. *Assume that $A_0(\lambda)$ is a constant matrix. Then, for all $\lambda \in \rho$, the corresponding Birman–Schwinger operator $\mathcal{K}(\lambda) = |V|\mathcal{K}_0(\lambda)\widetilde{V}^{1/2}$ is of trace class.*

Proof. Let $\kappa_l \coloneqq \kappa_l^{\pm}(\lambda),\ l = 1, \dots, 2n$, be the eigenvalues of $A_0(\lambda)$ for all $\lambda \in \rho$. For clarity, we first suppose that $P = P(\lambda)$ diagonalises $A_0(\lambda)$, i.e.

$$P^{-1}A_0(\lambda)P = \Pi_0(\lambda),$$

and we refer to Remark 4.3 below for the case $A_0(\lambda)$ is not diagonalisable. For all $\lambda \in \rho$, let $\hat{k}_0$ denote the Fourier transform of $\mathcal{K}_0$. Then, for all $\xi \in \mathbb{R}$, we have

$$\begin{aligned}
\hat{k}_0(\xi, \lambda) &= \big(i\xi \mathrm{id}_{2n} - A_0(\lambda)\big)^{-1} \\
&= P\big(i\xi \mathrm{id}_{2n} - \Pi_0(\lambda)\big)^{-1}P^{-1} \\
&= P \begin{pmatrix} (i\xi - \kappa_1)^{-1} & 0 \cdots & 0 \\ 0 & (i\xi - \kappa_2)^{-1} \cdots & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 \cdots & (i\xi - \kappa_{2n})^{-1} \end{pmatrix} P^{-1} \\
&= \det{}_{\mathbb{C}^{2n}}\Big(\big(i\xi \mathrm{id}_{2n} - A_0(\lambda)\big)^{-1}\Big) \times PB(\xi, \lambda)P^{-1},
\end{aligned}$$

where $B(\xi, \lambda)$ is defined as the matrix

$$\begin{pmatrix} \prod\limits_{l \neq 1}(i\xi - \kappa_l) & 0 \cdots & 0 \\ 0 & \prod\limits_{l \neq 2}(i\xi - \kappa_l) \cdots & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 \cdots & \prod\limits_{l \neq 2n}(i\xi - \kappa_l) \end{pmatrix}.$$

Consider the decomposition of $\mathcal{K}_0(\lambda)$ as $\mathcal{K}_0(\lambda) = \big(\mathcal{K}_0^{(1)}\mathcal{K}_0^{(2)}\big)(\lambda)$, where the operators $\mathcal{K}_0^{(1)}(\lambda)$ and $\mathcal{K}_0^{(2)}(\lambda)$ are defined through their Fourier transforms by

$$\hat{k}_0^{(1)}(\xi,\lambda) = \det_{\mathbb{C}^{2n}}\Big(\big(i\xi\mathrm{id}_{2n} - A_0(\lambda)\big)^{-1}\Big) \quad \text{and} \quad \hat{k}_0^{(2)}(\xi,\lambda) = PB(\xi,\lambda)P^{-1}. \tag{4.23}$$

The operator $\mathcal{K}_0^{(1)}(\lambda)$ is an integral operator defined in $L^2(\mathbb{R},\mathbb{C})$, and $\mathcal{K}_0^{(2)}(\lambda)$ is a closed operator from a subset of $H^1(\mathbb{R},\mathbb{C}^{2n})$ to $L^2(\mathbb{R},\mathbb{C}^{2n})$. Indeed, the domain of $\mathcal{K}_0^{(2)}(\lambda)$ follows from the fact that $\operatorname{dom}\mathcal{K}_0^{(2)}(\lambda) \subset L^2(\mathbb{R},\mathbb{C}^{2n})$ and also from the fact that, when $n = 1$, $\operatorname{dom}\mathcal{K}_0^{(2)}(\lambda) = H^1(\mathbb{R},\mathbb{C}^2)$ since $\mathcal{K}_0^{(2)}(\lambda)$ is a differential operator similar to $\mathcal{T}_0(\lambda)$. Therefore, if $|V|^{1/2}\mathcal{K}_0^{(1)}(\lambda)\widetilde{V}$ is of trace class then $\mathcal{K}(\lambda)$ is of trace class, as well. This follows from (cf. equation (2.16) of Chapter 2)

$$\begin{aligned}\|\mathcal{K}(\lambda)\|_{\mathfrak{I}_1} &= \big\||V|^{1/2}\big(\mathcal{K}_0^{(1)}(\lambda)\mathcal{K}_0^{(2)}(\lambda)\big)\widetilde{V}\big\|_{\mathfrak{I}_1} \\ &\leqslant \big\||V|^{1/2}\mathcal{K}_0^{(1)}(\lambda)\widetilde{V}\big\|_{\mathfrak{I}_1}\big\||V|^{1/2}\mathcal{K}_0^{(2)}(\lambda)\widetilde{V}\big\|. \end{aligned}\tag{4.24}$$

where $\|\cdot\|$ is the operator norm. To show that the operator $|V|^{1/2}\mathcal{K}_0^{(1)}(\lambda)\widetilde{V}$ is of trace class, observe that

$$\hat{k}_0^{(1)}(\xi,\lambda) = \prod_{j=1}^{2n}(\kappa_j - i\xi)^{-1}. \tag{4.25}$$

Therefore,

$$\begin{aligned}\big|\hat{k}_0^{(1)}(\xi,\lambda)\big| &\leqslant \prod_{j=1}^{2n}|\kappa_j - i\xi|^{-1} \\ &\leqslant \big(\max_{j=1,\ldots,2n}\{|\kappa_j - i\xi|^{-1}\}\big)^{2n} \\ &\leqslant |\kappa_* - i\xi|^{-2}, \end{aligned}\tag{4.26}$$

where $\kappa_* = \min_{j=1,\ldots,2n}\{|\kappa_j|\}$. For $n \geqslant 1$, it then follows from the last estimate and $|V|^{1/2}, \widetilde{V} \in L^2$ (cf. (4.6) and (4.20)) that $|V|^{1/2}\mathcal{K}_0^{(1)}(\lambda)\widetilde{V}$ is of trace class. Hence by Proposition 4.1, $\mathcal{K}(\lambda)$ is of trace class. □

Remark 4.3. When the matrix $A_0(\lambda)$ is not diagonalisable (cf. [47]), we write it in the Jordan form and the above proof remains the same. The only change is in the

entries of the matrix $B(\xi,\lambda)$ which are given by

$$\prod_{\substack{j=1\\ l\neq j}}^{2n}(i\xi-\kappa_j)\widetilde{J}_l(\xi,\lambda),$$

where the $\widetilde{J}_l(\xi,\lambda)$ are the upper triangular matrices of the block matrices $(i\xi\mathrm{id}_{2n}-J_l(\lambda))^{-1}$ with J_l as Jordan segments.

Remark 4.4. Since $\mathfrak{I}_p$ are two-sided operator ideals in the set of bounded linear operators (cf. equation (2.16)), we have, under the closedness assumption of the operator $\mathcal{T}_0(\lambda)$, that (cf. equation (4.24))

$$|V|^{1/2}\mathcal{K}_0^{(1)}(\lambda)\widetilde{V}\in\mathfrak{I}_p \quad \text{implies that} \quad \mathcal{K}(\lambda)\in\mathfrak{I}_p.$$

Suppose that $\mathcal{T}_0(\lambda)$ is derived from a scalar problem. Then the integral operator $\mathcal{K}_0^{(1)}(\lambda)$ is precisely the resolvent operator associated with the scalar problem, i.e., $\mathcal{K}_0^{(1)}(\lambda)=\big(\mathcal{L}_0-\lambda\mathrm{id}\big)^{-1}$, where $\mathcal{L}_0$ is a constant-coefficient differential operator. This can be seen when considering the scalar eigenvalue problem $\mathcal{L}_0u=\lambda u$, where for $a_j\in\mathbb{R}$,

$$\mathcal{L}_0=\sum_{j=0}^{2n}a_j\mathrm{d}^j/\mathrm{d}x^j \tag{4.27}$$

is defined in $L^2(\mathbb{R},\mathbb{C})$ with domain $H^{2n}(\mathbb{R},\mathbb{C})$. The Fourier transform of $\big(\mathcal{L}_0-\lambda\mathrm{id}\big)^{-1}$, which is $\prod_{j=1}^{2n}(\kappa_j-i\xi)^{-1}$, is exactly equal to $\hat{k}_0(\xi,\lambda)$, up to nonvanishing constant. Therefore, if the integral operator corresponding to the scalar problem is of trace class, so is the Birman–Schwinger operator $\mathcal{K}$ corresponding to the first order system. We summarise the result in a proposition.

Proposition 4.2. *Let the Birman–Schwinger operator $\mathcal{K}(\lambda)$ be derived from the scalar problem $(\mathcal{L}_0+v-\lambda\mathrm{id})u=0$, where $v\in L^1$. If the integral operator corresponding to the scalar problem is of trace class, so is $\mathcal{K}(\lambda)$.*

For general matrix-valued function A_0, let us assume that $\mathcal{K}(\lambda)$ is of trace class. Then we state the conditions under which one can compute its trace in terms of its kernel function $k(x,y;\lambda)$ which a-priori is discontinuous. We start by introducing the

following notation

$$\Phi = \begin{pmatrix} Y_0^- & Y_0^+ \end{pmatrix},$$

$$\Phi^{-1} = \begin{pmatrix} Z_0^+ \\ Z_0^- \end{pmatrix},$$

where $Y_0^- \in L^2(\mathbb{R}_-, \mathbb{C}^{2n\times r})$ and $Y_0^+ \in L^2(\mathbb{R}_+, \mathbb{C}^{2n\times(2n-r)})$ satisfy (4.13), and $Z_0^+ \in L^2(\mathbb{R}_+, \mathbb{C}^{r\times 2n})$ and $Z_0^- \in L^2(\mathbb{R}_-, \mathbb{C}^{(2n-r)\times 2n})$ satisfy the adjoint problem of (4.13) with r as the rank of the projection operator Q given in (4.14). Then with O denoting the null matrix, we have

$$\Phi Q = \begin{pmatrix} O & Y_0^- \end{pmatrix}, \qquad (\mathrm{id} - Q)\Phi^{-1} = \begin{pmatrix} Z_0^- \\ O \end{pmatrix}, \quad \text{for} \quad x \leqslant 0, \tag{4.28}$$

$$\Phi(\mathrm{id} - Q) = \begin{pmatrix} Y_0^+ & O \end{pmatrix}, \qquad Q\Phi^{-1} = \begin{pmatrix} O \\ Z_0^+ \end{pmatrix}, \quad \text{for} \quad x \geqslant 0, . \tag{4.29}$$

Since $\Phi(x,\lambda)\Phi^{-1}(x,\lambda) = \Phi^{-1}(x,\lambda)\Phi(x,\lambda) = \mathrm{id}_{2n}$, it follows that

$$Y_0^- Z_0^+ + Y_0^+ Z_0^- = \mathrm{id}_{2n}, \tag{4.30}$$

and

$$\begin{aligned} Z_0^+ Y_0^- &= \mathrm{id}_r, \\ Z_0^- Y_0^+ &= \mathrm{id}_{2n-r}, \\ Z_0^+ Y_0^+ &= O_{(2n-r)\times r}, \\ Z_0^- Y_0^- &= O_{r\times(2n-r)}. \end{aligned} \tag{4.31}$$

Thus

$$\begin{aligned} Y_0^-(x,\lambda) Z_0^+(y,\lambda) &= \Phi(x,\lambda) Q \Phi^{-1}(y,\lambda), \\ Y_0^+(x,\lambda) Z_0^-(y,\lambda) &= \Phi(x,\lambda)(\mathrm{id}_{2n} - Q)\Phi^{-1}(y,\lambda). \end{aligned} \tag{4.32}$$

Since $\mathcal{K}(\lambda)$ is of trace class, we explicitly have (cf. [30, Theorem 3.2] and [32, Theorem 4.1, Chap XIV])

$$\operatorname{tr}\mathcal{K}(\lambda) = \int_{\mathbb{R}} \operatorname{tr}_{\mathbb{C}^{2n}}\big(\pm Y_0^{\pm}(x,\lambda)Z_0^{\mp}(x,\lambda)V(x)\big)\mathrm{d}x. \tag{4.33}$$

The above equation is obtained after substituting the left-hand side of (4.32) in the expression of the kernel k in (4.18), and using the invariance of trace for a cyclic rotation of three matrices. From equation (4.30), an immediate consequence of the above equality is

$$\int_{\mathbb{R}} \operatorname{tr}_{\mathbb{C}^{2n}} V(x)\mathrm{d}x = 0.$$

Let us assume that V is continuous and that

$$\int_0^{\pm\infty} \operatorname{tr}_{\mathbb{C}^{2n}} V(x)\mathrm{d}x = 0. \tag{4.34}$$

Then the trace of $\mathcal{K}$ in terms of its kernel k is given by

$$\operatorname{tr}\mathcal{K}(\lambda) = \int_{\mathbb{R}} \operatorname{tr}_{\mathbb{C}^{2n}} k(x,x,\lambda)\mathrm{d}x. \tag{4.35}$$

Indeed, observe that

$$\begin{aligned}
\int_{\mathbb{R}} \operatorname{tr}_{\mathbb{C}^{2n}} k(x,x,\lambda)\mathrm{d}x &= \int_0^{+\infty} \operatorname{tr}_{\mathbb{C}^{2n}} |V(x)|^{1/2} Y_0^{+}(x,\lambda)Z_0^{-}(x,\lambda)\widetilde{V}(x)\mathrm{d}x \\
&\quad - \int_{-\infty}^0 \operatorname{tr}_{\mathbb{C}^{2n}} |V(x)|^{1/2} Y_0^{-}(x,\lambda)Z_0^{+}(x,\lambda)\widetilde{V}(x)\mathrm{d}x \\
&= \int_0^{\pm\infty} \operatorname{tr}_{\mathbb{C}^{2n}} |V(x)|^{1/2} (\mathrm{id}_{2n} - Y_0^{\mp}(x,\lambda)Z_0^{\pm}(x,\lambda))\widetilde{V}(x)\mathrm{d}x \\
&\quad - \int_{\mp\infty}^0 \operatorname{tr}_{\mathbb{C}^{2n}} |V(x)|^{1/2} Y_0^{\mp}(x,\lambda)Z_0^{\pm}(x,\lambda)\widetilde{V}(x)\mathrm{d}x \\
&= \int_0^{\pm\infty} \operatorname{tr}_{\mathbb{C}^{2n}} V(x)\mathrm{d}x + \int_{\mathbb{R}} \operatorname{tr}_{\mathbb{C}^{2n}}\big(\pm Y_0^{\pm}(x,\lambda)Z_0^{\mp}(x,\lambda)V(x)\big)\mathrm{d}x.
\end{aligned}$$

Using (4.30) and (4.34), the trace of $\mathcal{K}$ in (4.35) follows. Note that any Green's function associated with the first order system of differential equations is discontinuous on the diagonal (jump condition, cf. Theorem 4.1). With the condition (4.34), one

expresses the trace of the corresponding Birman–Schwinger operator $\mathcal{K}(\lambda)$ in terms of its kernel. Therefore, the right-hand side of (4.35) can be viewed as a generalisation of integral trace for trace class operators which do not have continuous kernels, in particular.

Remark 4.5. We claim that in addition to the continuity of the perturbation V, if the diagonal elements of V are equal to zero, the integral kernel k is continuous. To see this, consider for example a Schrödinger problem rewritten as a first order system of differential equations

$$\frac{\mathrm{d}}{\mathrm{d}x}Y = \big(A_0(\lambda) + V(x)\big)Y,$$

where

$$A_0(\lambda) = \begin{pmatrix} 0 & 1 \\ \kappa^2 & 0 \end{pmatrix} \quad \text{and} \quad V = \begin{pmatrix} 0 & 0 \\ v & 0 \end{pmatrix}$$

with v continuous in L^1. Then the kernel of the Birman–Schwinger operator $\mathcal{K}(\lambda)$ is given by

$$k(x,y;\kappa) = \frac{1}{2\kappa}\begin{cases} -|V(x)|^{1/2}\begin{pmatrix} \kappa \mathrm{e}^{\kappa(x-y)} & \mathrm{e}^{\kappa(x-y)} \\ \kappa^2 \mathrm{e}^{\kappa(x-y)} & \kappa \mathrm{e}^{\kappa(x-y)} \end{pmatrix} \widetilde{V}(y), & x \leqslant y \\ |V(x)|^{1/2}\begin{pmatrix} \kappa \mathrm{e}^{-\kappa(x-y)} & -\mathrm{e}^{-\kappa(x-y)} \\ -\kappa^2 \mathrm{e}^{\kappa(x-y)} & \kappa \mathrm{e}^{-\kappa(x-y)} \end{pmatrix} \widetilde{V}(y), & x > y \end{cases}$$

$$= \frac{1}{2\kappa}\begin{pmatrix} |v(x)|^{1/2}\mathrm{e}^{-\kappa|x-y|}v(y)/|v(y)|^{1/2} & 0 \\ 0 & 0 \end{pmatrix},$$

where

$$|V|^{1/2} = \begin{pmatrix} |v|^{1/2} & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \widetilde{V} = \begin{pmatrix} 0 & 0 \\ v/|v|^{1/2} & 0 \end{pmatrix}.$$

We can see that the kernel k is continuous and its corresponding Birman–Schwinger operator $\mathcal{K}(\lambda)$ is of trace class (cf. Theorem 4.2 or Proposition 4.2 with [66] and [25]). We shall prove our claim for systems deriving from scalar problems of higher order in the next subsection.

4.1.2 A class of travelling wave problem

We consider a class of eigenvalue problems that arise in the stability analysis of travelling waves. In this class which includes for example the generalised or regularised Boussinesq equation, (generalised) Korteweg–de Vries equation, the fifth-order KdV equation, (generalised) Benjamin–Bona–Mahoney equation and so on, the corresponding first order system of the differential operator $\mathcal{T}_0(\lambda)$ has constant coefficients. We restrict our attention to the scalar case. However, we might use the corresponding first order system formulation, if required. Our objective is to show that the corresponding Birman–Schwinger operators are of trace class. We consider perturbations given as differential operators with smooth coefficients belonging to $L^1(\mathbb{R})$.

Let the differential operator associated with our eigenvalue problem

$$\mathcal{L}\colon H^n(\mathbb{R},\mathbb{C}) \to L^2(\mathbb{R},\mathbb{C})$$

be given by

$$\mathcal{L} = \mathcal{L}_0 + v, \tag{4.36}$$

where $n \geqslant 2$, $\mathcal{L}_0$ is an nth order ordinary differential operator with constant coefficients (cf. (4.27)), and for $m = 0, \ldots, n-2$,

$$v = \sum_{i=0}^{m} \phi_i(x) \frac{\mathrm{d}^i}{\mathrm{d}x^i} \tag{4.37}$$

with

$$\phi_i = \binom{m}{i} \frac{\mathrm{d}^{m-i}}{\mathrm{d}x^{m-i}} \phi. \tag{4.38}$$

The above perturbation arises in the study of KdV equations, for example. Note that the range of m in (4.37) is suitably chosen so that no jump discontinuity occurs on the diagonal of the Green's function associated with $\big(\mathcal{L}_0 - \lambda \mathrm{id}\big)$.

For all $\lambda \in \rho$, let

$$P_n(\kappa) = \kappa^n + a_{n-1}\kappa^{n-1} + \ldots + a_1\kappa + a_0 - \lambda \tag{4.39}$$

be the characteristic polynomial associated with $(\mathcal{L}_0 - \lambda\mathrm{id})$.

In what follows, we shall assume the following hypothesis.

Hypothesis 4.1. *Assume that the roots of $P_n(\lambda)$ are simple and have nonzero real parts.*

We denote by $\kappa_j^+,\ j = 1, \ldots, r$, the roots with positive real parts, and by $\kappa_j^-,\ j = r+1, \ldots, n$, the roots with negative real parts. Under Hypothesis 4.1, the operator $(\mathcal{L}_0 - \lambda\mathrm{id})$ is Fredholm. Therefore, the Green's function g_0 of the resolvent operator $(\mathcal{L}_0 - \lambda\mathrm{id})^{-1}$ is given, for all $x, y \in \mathbb{R}$ and $\lambda \in \rho$, by

$$g_0(x, y; \lambda) = \begin{cases} \sum_{j=1}^{r} \alpha_j^+ \mathrm{e}^{\kappa_j^+(x-y)}, & x \leqslant y \\ \sum_{j=1}^{n-r} \alpha_j^- \mathrm{e}^{\kappa_j^-(x-y)}, & y < x, \end{cases} \tag{4.40}$$

where $\alpha_j = \alpha_j^{\pm}(\lambda) \in \mathbb{C}$. The coefficients $\alpha_j^{\pm}$ satisfy the following matrix equation

$$\begin{pmatrix} 1 & \ldots & 1 & -1 & \ldots & -1 \\ \kappa_1^+ & \ldots & \kappa_k^+ & -\kappa_{k+1}^- & \ldots & -\kappa_n^- \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ (\kappa_1^+)^{n-1} & \ldots & (\kappa_k^+)^{n-1} & -(\kappa_{k+1}^-)^{n-1} & \ldots & -(\kappa_n^-)^{n-1} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ -1 \end{pmatrix}. \tag{4.41}$$

Note that since $(\mathcal{L}_0 - \lambda\mathrm{id})$ is a constant coefficient differential operator, the projection Q is constant. From the previous subsection, the eigenvalue problem associated with the operator $\mathcal{L}$ reduces to an integral eigenvalue problem given, for all $\lambda \in \rho$ and $u \in L^2$, by

$$u = (\mathcal{L}_0 - \lambda\mathrm{id})^{-1} v u. \tag{4.42}$$

With integration by parts, the above equation becomes

$$u(x) = (-1)^{m+1} \int_{\mathbb{R}} \left(\partial_y^m g_0(x, y; \lambda)\right) \phi(y) u(y)\, \mathrm{d}y, \tag{4.43}$$

where the Green's function g is given in (4.40), and $u(x) \coloneqq u(x, \lambda)$. Note that the factor $(-1)^m$ in the above equation is multiplied by that of the mth derivative of g_0 with respect to y, $\partial_y^m g_0$. We set $\psi \coloneqq |\phi|^{1/2} u$ and $\tilde{\phi} \coloneqq \phi/|\phi|^{1/2}$. Then the integral

equation (4.43) is equivalent, for all $\lambda \in \rho$ and $\psi \in L^2$, to

$$\Big(\mathrm{id} + \mathcal{G}_m(\lambda)\Big)\psi = 0,$$

where the Birman–Schwinger operator $\mathcal{G}_m(\lambda)$ is given by

$$\mathcal{G}_m(\lambda) = |\phi|^{1/2}\mathcal{G}_m^{(0)}(\lambda)\tilde{\phi}, \tag{4.44}$$

with $\mathcal{G}_m^{(0)}(\lambda)$ the resolvent operator associated with the kernel function $\partial_y^m g_0$. Explicitly, the kernel g_m associated with $\mathcal{G}_m(\lambda)$ is given, for all $\lambda \in \rho$, by

$$g_m(x,y;\lambda) = \begin{cases} |\phi(x)|^{1/2} \sum\limits_{j=1}^{r} (\kappa_j^+)^m \alpha_j^+ \mathrm{e}^{\kappa_j^+(x-y)}\tilde{\phi}(y), & x \leqslant y \\ |\phi(x)|^{1/2} \sum\limits_{j=r+1}^{n} (\kappa_j^-)^m \alpha_j^- \mathrm{e}^{\kappa_j^-(x-y)}\tilde{\phi}(y), & y < x. \end{cases} \tag{4.45}$$

Observe that the kernel $g_m \in L^2(\mathbb{R}^2 \times \rho, \mathbb{C})$ and so $\mathcal{G}_m(\lambda)$ are of Hilbert–Schmidt class, for all m. Indeed, since the Green's function $\partial_y^m g_0$ is continuous for all $x, y \in \mathbb{R}$, $\lambda \in \rho$ and $m = 0, \ldots (n-2)$, and $\phi \in L^1$, then following the computational steps in (4.21), we arrive at the conclusion.

Proposition 4.3. *For a general constant coefficient operator $\mathcal{L}_0 - \lambda\mathrm{id}$, where the roots of its characteristic polynomial $P_n(\kappa)$ have non-zero real parts, the Birman–Schwinger operator $\mathcal{G}_m(\lambda)$ is of trace class, for all $\lambda \in \rho$ and $m = 0, \ldots, (n-2)$.*

Proof. For all $\lambda \in \rho$ and $m = 0, \ldots, (n-2)$, let us denote by $\hat{g}_m$ the Fourier transform of the resolvent operator $\mathcal{G}_m^{(0)}(\lambda)$. For $m = 0$, the Fourier transform $\hat{g}_0$ of the resolvent operator $\mathcal{G}_0^{(0)}(\lambda)$ is equal to $1/P_n(i\xi)$, where P_n is defined in (4.39). By Hypothesis 4.1, $\hat{g}_0$ satisfies the following

$$\begin{aligned} |\hat{g}_0(\xi,\lambda)| &\leqslant \prod_{j=1}^{n} |\kappa_j - i\xi|^{-1} \\ &\leqslant |\kappa_* - i\xi|^{-2} \end{aligned}$$

where κ_* is given in (4.26). For $m = 0, \ldots, (n-2)$, there is some nonvanishing constant

c_m depending on λ, such that the Fourier transform $\hat{g}_m$ satisfies the following

$$\begin{aligned}\hat{g}_m(\xi,\lambda) &= \int_{\mathbb{R}} \partial_x^m g_0(x,\lambda)\mathrm{e}^{-i\xi x}\mathrm{d}x \\ &= c_m(\lambda)\int_{\mathbb{R}} g_0(x,\lambda)\mathrm{e}^{-i\xi x}\mathrm{d}x \\ &= c_m(\lambda)\hat{g}_0(\xi,\lambda).\end{aligned}$$

Hence by the above inequality and Proposition 4.1, the $\mathcal{G}_m(\lambda)$ are of trace class, for all $\lambda \in \rho$ and $m = 0,\ldots,(n-2)$. □

Remark 4.6. Note that for a general constant coefficient differential operator $\mathcal{L}_0 - \lambda\mathrm{id}$, the Green's function g_0 is not usually in the form given in (4.40).

Since $\mathcal{G}_m(\lambda)$ are of trace class, the corresponding Fredholm determinants are given by

$$\det_1\big(\mathrm{id} + \mathcal{G}_m(\lambda)\big) = 1 + \sum_{l=1}^{\infty} d_l(\lambda), \tag{4.46}$$

where

$$d_l(\lambda) = \frac{1}{l!}\int_{\mathbb{R}}\cdots\int_{\mathbb{R}} \det_{\mathbb{C}^l}\big([g_m(x_i,x_j;\lambda)]_{i,j=1,\ldots,l}\big)\mathrm{d}x_1\cdots\mathrm{d}x_l. \tag{4.47}$$

For all $\lambda \in \rho$ and $m = 0,\ldots(n-2)$, the function $\partial_y^m g_0$ is continuous in $\mathbb{R}\times\mathbb{R}$, and in particular, on the diagonal $x = y$, thus

$$\sum_{j=r+1}^{n} (\kappa_j^-)^m \alpha_j = \sum_{j=1}^{r} (\kappa_j^+)^m \alpha_j.$$

When $l = 1$ in (4.47), we have

$$\begin{aligned}d_1(\lambda) &= \mathrm{tr}\,\mathcal{G}_m(\lambda) \\ &= \int_{\mathbb{R}} g_m(x,x;\lambda)\mathrm{d}x \\ &= \sum_{j=1}^{r}(\kappa_j^+)^m\alpha_j\int_{\mathbb{R}}\phi(x)\mathrm{d}x \\ &= \sum_{j=r+1}^{n}(\kappa_j^-)^m\alpha_j\int_{\mathbb{R}}\phi(x)\mathrm{d}x.\end{aligned}$$

The claim in Remark 4.5, suggesting the continuity of the Birman–Schwinger kernel k associated with the system, can now be proved. Rewrite the eigenvalue problem as a first order system of differential equations, where the perturbation

$$V = \begin{pmatrix} O & O \\ v_m & O \end{pmatrix} \tag{4.48}$$

with O as the zero matrix of appropriate size and $v_m = (\phi_0, \cdots, \phi_m)$, and

$$A_0(\lambda) = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & & 0 \\ 0 & 0 & & & 1 \\ \lambda - a_0 & -a_1 & & \cdots & -a_{n-1} \end{pmatrix}.$$

By Proposition 4.2, the corresponding Birman–Schwinger operator $\mathcal{K}$ for the system is of trace class. Note that since $\operatorname{tr}_{\mathbb{C}^n} V = 0$ in (4.48), and that the Jordan-block structures of the operators $(\mathcal{L} - \lambda\mathrm{id})$ (resp. $\mathcal{L}_0 - \lambda\mathrm{id}$) and $\mathcal{T}(\lambda)$ (resp. $\mathcal{T}_0(\lambda)$) are the same (cf. [64, Example 1 (continued)]),

$$\begin{aligned} \operatorname{tr} \mathcal{K}(\lambda) &= \int_{\mathbb{R}} \operatorname{tr}_{\mathbb{C}^n} k(x, x; \lambda) \mathrm{d}x \\ &= \int_{\mathbb{R}} g_m(x, x; \lambda) \mathrm{d}x \\ &= \operatorname{tr} \mathcal{G}_m(\lambda). \end{aligned}$$

To show the continuity of the kernel k, one needs to show, for all $x \in \mathbb{R}$ and $\lambda \in \rho$, that $\operatorname{tr}_{\mathbb{C}^n} k(x, x; \lambda) = g_m(x, x; \lambda)$. To this end, it is sufficient to show that it is true for $m = 0$ since $g_m(x, x, \lambda) = c_m(\lambda) g_0(x, x, \lambda)$. We write the kernel k as follows

$$k = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix},$$

where, for $l, j = 1, 2,\ n_1 = r$ and $n_2 = n - r,\ k_{lj} \in \mathbb{C}^{n_l \times n_j}$. Moreover, we write

$$|V|^{1/2} = \operatorname{diag}\left(|\phi|^{1/2}, 0, \cdots, 0\right) \quad \text{and} \quad \widetilde{V} = \begin{pmatrix} O & O \\ \phi|\phi|^{-1/2} & O \end{pmatrix}. \tag{4.49}$$

It follows that

$$\Psi = |V|^{1/2} Y = \begin{pmatrix} |\phi|^{1/2} u & 0 & \cdots & 0 \end{pmatrix}^T.$$

Given the sparse structure of the matrix-valued functions $|V|^{1/2}$ and $\widetilde{V}$ in (4.49), we have that the block matrices k_{12}, k_{21} and k_{22} are identically zero. The only nonzero entry in the $r \times r$ block matrix k_{11} is the top level entry $g_0(x, y; \lambda)$ (since $|\phi|^{1/2} u \neq 0$ and $\Psi = (|\phi|^{1/2} u, 0, \ldots, 0)^T = \mathcal{K}(\lambda)\Psi$, it follows that the first entry $\mathcal{G}_0(\lambda)$ is the only nonzero operator in $\mathcal{K}(\lambda)$), for all $x, y \in \mathbb{R}$ and $\lambda \in \rho$. Hence, we have

$$k(x, y; \lambda) = \operatorname{diag}\left(g_0(x, y; \lambda),\ 0, \cdots, 0\right).$$

Consequently, the continuity of k follows.

Now assume that ϕ_i do not have the form given in (4.38). Then we proceed by integration by parts to avoid an integro-differential equation in (4.42). If not, the computation of the determinant can be difficult. Alternatively, suppose that the left inverse of $\mathcal{L}_0 - \lambda\mathrm{id}$ exists. Then from Subsection 4.1.1, we have, for all $\lambda \in \rho$ and $u \in L^2$,

$$\left(\mathrm{id} + v(\mathcal{L}_0 - \lambda\mathrm{id})^{-1}\right) u = 0. \tag{4.50}$$

For $m = 0, \ldots, (n-2)$, the kernel function of $v(\mathcal{L}_0 - \lambda\mathrm{id})^{-1}$ is

$$\sum_{j=0}^{m} \phi_j(x) \partial_x^j g_0(x, y; \lambda),$$

where g_0 is the Green's function associated with the differential operator $(\mathcal{L}_0 - \lambda\mathrm{id})$. Let $\widetilde{\mathcal{G}}_m(\lambda)$ denote the Birman–Schwinger operator when ϕ_i is of general form. We claim that the determinant of $\left(\mathrm{id} + v(\mathcal{L}_0 - \lambda\mathrm{id})^{-1}\right)$ is equal to the determinant of $\left(\mathrm{id} + \widetilde{\mathcal{G}}_m(\lambda)\right)$, up to a nonvanishing analytic function. Indeed when $m = 0$, the coefficients in the Fredholm determinant series (cf. equation. (4.47)) associated with both operators $\widetilde{\mathcal{G}}_m(\lambda)$ and $v(\mathcal{L}_0 - \lambda\mathrm{id})^{-1}$ are equal. Hence, the zeros of $\det_p\big(\mathrm{id} +$

$v(\mathcal{L}_0 - \lambda\mathrm{id})^{-1}\big)$ coincide in order (location) to algebraic multiplicity of eigenvalues of $\mathcal{L}$. Thus one can choose either one of the determinants for computing eigenvalues of $\mathcal{L}$.

The pure point spectrum of a constant coefficient differential operator is empty (cf. [21]). Therefore, the resolvent set ρ of the operator $\mathcal{L}_0$ is given by

$$\rho = \mathbb{C} \setminus \sigma_e(\mathcal{L}_0), \tag{4.51}$$

where the *essential spectrum* $\sigma_e(\mathcal{L}_0)$ is the complement of the pure point spectrum in $\sigma(\mathcal{L}_0)$. Due to the invariance of essential spectra under compact perturbation, the essential spectra of $\mathcal{L}_0$ and $\mathcal{L}$ coincide, and it is given by

$$\sigma_e(\mathcal{L}_0) = \mathrm{closure}(\big\{\lambda \in \mathbb{C}\colon \lambda = \sum_{j=0}^{n} a_j (i\xi)^j, \quad \xi, a_j \in \mathbb{R}\big\}),$$

or, equivalently

$$\sigma_e(\mathcal{L}_0) = \mathrm{closure}(\{\lambda \in \mathbb{C}\colon \det_{\mathbb{C}^n}\big(A_0(\lambda) - i\xi\mathrm{id}\big) = 0,\ \xi \in \mathbb{R}\}).$$

Note that $\lambda = 0$ is an eigenvalue of the operator $\mathcal{L}$ which is embedded in the essential spectrum, since $\lim_{|x|\to\infty} v(x) = 0$.

4.2 The Evans function

In this section, we show that the Evans function is proportional to a finite dimensional determinant associated with a matrix of length r or $n - r$.

The *(matrix-valued) Jost solution* (cf. [69] and [28])) is an analytic solution in $\lambda \in \rho$ of $\mathcal{T}(\lambda)Y = 0$ which is asymptotically close to a square integrable solution of $\mathcal{T}_0(\lambda)Y = 0$, at infinity.

Definition 4.2. Assume that the matrix-valued Jost solutions exist. Then for all $\lambda \in \rho$, we define the *matrix transmission coefficient* $D(\lambda)$ by

$$D(\lambda) \coloneqq \lim_{x\to+\infty} Z_0^+(x,\lambda)Y^-(x,\lambda) \tag{4.52}$$

where Z_0^+ satisfies $\mathcal{T}_0^*(\lambda)Z_0^+ = 0$ and Y^- is the matrix-valued Jost solution which decays at $-\infty$, and satisfies $\mathcal{T}(\lambda)Y^- = 0$.

In what follows, we suppress the λ dependence in any concerned function, i.e. we simply write $Y(x) = Y(x, \lambda)$ for example.

For some appropriate $\beta > 0$, we consider matrix-valued Jost solutions of the following form (cf. [28] and [69])

$$Y^{\pm} = \mathrm{e}^{\mp\beta x}\widetilde{Y}^{\pm}, \tag{4.53}$$

where the matrix-valued solutions $\widetilde{Y}^{\pm}$ satisfy the following Volterra equations

$$\widetilde{Y}^{\pm}(x) = \mathrm{e}^{\pm\beta x}Y_0^{\pm}(x) - \int_x^{\pm\infty} \mathrm{e}^{\pm\beta(x-y)}\Phi(x)\Phi^{-1}(y)V(y)\widetilde{Y}^{\pm}(y)\mathrm{d}y \tag{4.54}$$

with $Y_0^{\pm}$ satisfying $\mathcal{T}_0(\lambda)Y_0^{\pm} = 0$, $\Phi = (Y_0^- \quad Y_0^+)$ a fundamental matrix solution and $\|V\|_{\mathbb{C}^{n\times n}} \in L^1(\mathbb{R}, \mathbb{C}, \mathrm{e}^{\beta|x|}\mathrm{d}x)$. For such a $\beta > 0$, the Jost solutions can be uniquely determined by solving the above equation without the exponential factors (see Gesztesy et al. [28]). In fact, they can be expressed as Neumann series since the Volterra operators defined in the above equation are of Hilbert–Schmidt class in $L^2(\mathbb{R}^{\pm}, \mathbb{C})$, for all $\lambda \in \rho$ and $\|V\|_{\mathbb{C}^{n\times n}} \in L^1(\mathbb{R}, \mathbb{C}, \mathrm{e}^{\beta|x|}\mathrm{d}x)$. Indeed, let us suppose that $\beta > \max\{\kappa, \kappa'\}$, where κ, κ' are introduced in the definition of the exponential dichotomy in (4.14). Then for all $x \leqslant 0$, using the inequalities in (4.14) and writing the matrix norm $\|\cdot\| = \|\cdot\|_{\mathbb{C}^{n\times n}}$, it follows, for some constant $c(\kappa, \kappa') > 0$, that

$$\begin{aligned}
\int_{-\infty}^{x} \big\|\Phi(x)\Phi^{-1}(y)V(y)\big\|\mathrm{d}x &= \int_{-\infty}^{x} \big\|(\Phi(x)Q\Phi^{-1}(y) + \Phi(x)(\mathrm{id}_n - Q)\Phi^{-1}(y))V(y)\big\|\mathrm{d}y \\
&\leqslant c(\kappa', \kappa)\int_{-\infty}^{x} \mathrm{e}^{\kappa'(x-y)}\|V(y)\|\mathrm{d}y \\
&\leqslant c(\kappa', \kappa)\int_{-\infty}^{x} \mathrm{e}^{\kappa' x}\mathrm{e}^{(\beta-\kappa')y}\mathrm{d}y < \infty.
\end{aligned} \tag{4.55}$$

For all $x \geqslant y$, we use $\mathrm{e}^{\kappa'(x-y)} + \mathrm{e}^{-\kappa(x-y)} \leqslant 2\mathrm{e}^{\kappa'(x-y)}$ in the second line of the above inequality. Observe that the last estimate implies the compactness of the Volterra operator, for all $x \leqslant 0$. We remark that our assumption on β is quite stronger than that given in Gesztesy et al. [28].

Remark 4.7. 1. In our case, β is such that the following inequality holds

$$\begin{aligned}\left\|\Phi(x)Q\Phi^{-1}(y)+\Phi(x)(\mathrm{id}_n-Q)\Phi^{-1}(y)\right\| &\leqslant c(\kappa')\mathrm{e}^{\kappa'(x-y)}+c(\kappa)\mathrm{e}^{-\kappa(x-y)}\\ &\leqslant c(\kappa',\kappa)\mathrm{e}^{\beta|x-y|}.\end{aligned}$$

Hence this implies that β must be chosen greater or equal to the $\max\{\kappa,\kappa'\}$.

2. If the strict inequality $\beta>\max\{\kappa,\kappa'\}$ is replaced by a less strict one, then from (4.55), the uniqueness of matrix-valued Jost solutions is not guaranteed.

3. The matrix-valued solutions $\widetilde{Y}^{\pm}$ in (4.54) satisfy the following differential equation
$$\frac{\mathrm{d}}{\mathrm{d}x}\widetilde{Y}^{\pm}=(A(x,\lambda)\pm\beta\mathrm{id}_n)\widetilde{Y}^{\pm}.$$

In the context of the Evans function, λ is an eigenvalue if the subspaces, defined by the set of solutions of $\mathcal{T}(\lambda)Y=0$ that decay at $\pm\infty$, have nontrivial intersection. In fact, this coincides with the geometric interpretation of Definition 4.2. That is, if for some $\lambda\in\rho$ and as x goes to ∞, the subspaces E^- and E^+_*, spanned respectively by the column vectors of Y^- and Z^-_0, are orthogonal, then the subspaces E^- and E^+_0 have nontrivial intersection. This is because for all $x\in\mathbb{R}$ and $\lambda\in\rho$, the subspaces E^+_0 (spanned by the column vectors of Y^+_0) and E^+_* are orthogonal. In other words, if for some $\lambda\in\rho$, the subspaces E^- and E^+ (spanned by the column vectors of Y^+) have nontrivial intersection, so do the subspaces E^- and E^+_0 as x tends to ∞.

Lemma 4.1. *Assume that* $\|V\|_{\mathbb{C}^{n\times n}}\in L^1(\mathbb{R},\mathbb{C},\mathrm{e}^{\beta|x|}\mathrm{d}x)$*, for some* $\beta>0$*. Then, for all* $\lambda\in\rho$*, the finite dimensional matrix* $D(\lambda)$ *in* (4.52) *satisfies*

$$\det_{\mathbb{C}^r}D(\lambda)=\lim_{x\to+\infty}\det_{\mathbb{C}^r}Z^+(x)Y^-(x), \tag{4.56}$$

where Z^+ *is the matrix-valued Jost solution of the adjoint problem, i.e. solution of*

$$Z^{\pm}(x)=Z^{\pm}_0(x)+\int_x^{\pm\infty}Z^{\pm}(y)V(y)H(y,x)\mathrm{d}y \tag{4.57}$$

decaying at $\pm\infty$ *with*

$$H(x,y)=Y^-_0(x)Z^+_0(y)+Y^+_0(x)Z^-_0(y)=\Phi(x)\Phi^{-1}(y). \tag{4.58}$$

Proof. Using equation (4.31) which resulted from the identity $\Phi(x)\Phi^{-1}(x) = \mathrm{id}_n$, the right-hand side of the matrix transmission coefficient (4.52) becomes

$$\begin{aligned} Z_0^+(x)Y^-(x) &= Z_0^+(x)\Big(Y_0^-(x) + \int_{-\infty}^{x} H(x,y)V(y)Y^-(y)\mathrm{d}y\Big) \\ &= \mathrm{id}_r + \int_{-\infty}^{x} Z_0^+(y)V(y)Y^-(y)\mathrm{d}y. \end{aligned} \tag{4.59}$$

Observe that the above equation is independent of the variable x. Therefore,

$$\det_{\mathbb{C}^r} D(\lambda) = \lim_{x\to+\infty} \det_{\mathbb{C}^r} Z_0^+(x)Y^-(x). \tag{4.60}$$

Substituting the matrix-valued Jost solution Y^- in the right-hand side of (4.56) and using again (4.31), it implies that

$$\begin{aligned} Z^+(x)Y^-(x) = Z_0^+(x)Y_0^-(x) &+ Z_0^+(x)\int_{-\infty}^{x} H(x,y)V(y)Y^-(y)\mathrm{d}y \\ &+ Y_0^-(x)\int_{x}^{+\infty} Z^+(y)V(y)H(y,x)\mathrm{d}y \\ &+ \int_{x}^{+\infty} Z^+(y)V(y)H(y,x)\mathrm{d}y \int_{-\infty}^{x} H(x,y)V(y)Y^-(y)\mathrm{d}y. \end{aligned}$$

Similarly, the above equation is independent of the variable x. Hence taking the limit as x goes ∞, the third and the fourth terms in the right-hand side of the above equation vanish, and so the result coincides with equation (4.60). Consequently, equation (4.56) in the above lemma follows. □

Hypothesis 4.2. *For all $\lambda \in \rho$, assume that $A_0(x,\lambda) = A_0(\lambda)$ is a constant-valued matrix.*

Remark 4.8. Under the above hypothesis, the exponential decay condition of the perturbation can be relaxed, i.e. $\|V\|_{\mathbb{C}^{n\times n}} \in L^1(\mathbb{R},\mathbb{C},(1+|x|)^q\mathrm{d}x)$ $(q>1)$ when $A_0(\lambda)$ is not diagonalisable and $\|V\|_{\mathbb{C}^{n\times n}} \in L^1$ otherwise (cf. [27, Section 8 and Theorem 8.3]).

Let the Evans function $E(\lambda)$ be given by

$$E(\lambda) = \det_{\mathbb{C}^n}\begin{pmatrix} Y^-(x) & Y^+(x)\end{pmatrix}, \tag{4.61}$$

where Y^- and Y^+ are the matrix-valued Jost solutions decaying at $\pm\infty$. Then the following result holds.

Theorem 4.3. *For all $\lambda \in \rho$, the Evans function $E(\lambda)$ and the determinant of the matrix transmission coefficient $D(\lambda)$ satisfy*

$$\det_{\mathbb{C}^r} D(\lambda) = \frac{E(\lambda)}{c(\lambda)}, \tag{4.62}$$

where $c(\lambda)$ is a nonvanishing analytic function.

Proof. For all $\lambda \in \rho$, we have

$$\begin{aligned} E(\lambda) = &\det_{\mathbb{C}^n} \begin{pmatrix} Y^-(x) & Y^+(x) \end{pmatrix} \\ = &\det_{\mathbb{C}^n} \begin{pmatrix} Y_0^-(x) & Y_0^+(x) \end{pmatrix} \\ &\det_{\mathbb{C}^n} \left(\mathrm{id} + \begin{pmatrix} Z_0^+(x) \\ Z_0^-(x) \end{pmatrix} \begin{pmatrix} \mathcal{H}^-(\lambda)Y^-(x) & \mathcal{H}^+(\lambda)Y^+(x) \end{pmatrix} \right), \end{aligned}$$

where the Volterra operators $\mathcal{H}^\pm(\lambda)$ are given by

$$\mathcal{H}^\pm(\lambda)Y^\pm(x) = -\int_x^{\pm\infty} H(x,y)V(y)Y^\pm(y)\mathrm{d}y$$

with H is given by (4.58). Using equation (4.31), it follows that

$$\begin{aligned} E(\lambda) = c(\lambda) \det_{\mathbb{C}^n} \Bigg[&\begin{pmatrix} \mathrm{id}_r & O \\ O & \mathrm{id}_{n-r} \end{pmatrix} \\ &+ \begin{pmatrix} \int_{-\infty}^x Z_0^+(y)V(y)Y^-(y)\mathrm{d}y & -\int_x^\infty Z_0^+(y)V(y)Y^+(y)\mathrm{d}y \\ \int_{-\infty}^x Z_0^-(y)V(y)Y^-(y)\mathrm{d}y & -\int_x^\infty Z_0^-(y)V(y)Y^+(y)\mathrm{d}y \end{pmatrix} \Bigg], \end{aligned} \tag{4.63}$$

where $c(\lambda) = \det_{\mathbb{C}^n} \begin{pmatrix} Y_0^-(x) & Y_0^+(x) \end{pmatrix}$. Note again that the integrands in the above equation are independent of the variable x. Hence taking the limit as x goes for example to ∞,

$$E(\lambda) = c(\lambda) \det_{\mathbb{C}^r} D(\lambda). \tag{4.64}$$

□

As a result of (4.64), the determinant of the matrix transmission coefficient $\det_{\mathbb{C}^r} D(\lambda)$ enjoys the same properties of the Evans function $E(\lambda)$—the zeros of $\det_{\mathbb{C}^r} D(\lambda)$ coincide in location and multiplicity to eigenvalue of $\mathcal{T}(\lambda)$.

Remark 4.9. The exponential factor in the expression of the Evans function $E(\lambda)$ in (4.61) is omitted because both $E(\lambda)$ and $c(\lambda)$ have the same trace.

Remark 4.10. Note that in the case the eigenvalues κ_j^+ or κ_j^- of $A_0(\lambda)$ are simple, the determinant of the matrix transmission coefficient $D(\lambda)$ is the Evans function $E_S(\lambda)$ in (3.12) of Chapter 3 (cf. [69] and [12]).

4.3 Regularised Fredholm determinants

In this section, we show that the p-regularised Fredholm determinants associated with $\mathcal{K}(\lambda)$ is equal to the determinant of the matrix transmission coefficient $D(\lambda)$, up to a nonvanishing analytic function. We start with the case $\mathcal{K}(\lambda)$ being of trace class. This will then facilitate the proof in case $\mathcal{K}(\lambda) \in \mathfrak{I}_p$, for $p \geqslant 2$.

4.3.1 Trace class operators

For all $\lambda \in \rho$, we assume that $\mathcal{K}(\lambda)$ is of trace class. Then the following result holds.

Theorem 4.4. *For all $\lambda \in \rho$, the determinant of the matrix transmission coefficient $D(\lambda)$ equals the Fredholm determinant, that is*

$$\det_{\mathbb{C}^r} D(\lambda) = \det_1\big(\mathrm{id} - \mathcal{K}(\lambda)\big).$$

Moreover, we have

$$\det_1\big(\mathrm{id} - \mathcal{K}(\lambda)\big) = \frac{E(\lambda)}{c(\lambda)}. \tag{4.65}$$

Proof. Taking the limit as $x \to \infty$ in (4.59), we have

$$\det_{\mathbb{C}^r} D(\lambda) = \det_{\mathbb{C}^r}\big(\mathrm{id}_r + M(\lambda)\big), \tag{4.66}$$

where

$$M(\lambda) = \int_{\mathbb{R}} Z_0^+(x) V(x) Y^-(x) \mathrm{d}x.$$

Since the finite rank operator $M(\lambda)$ is analytic in λ, then the finite dimensional determinant $\det_{\mathbb{C}^r}\big(\mathrm{id}_r + M(\lambda)\big)$, as well as, $\det_{\mathbb{C}^r} D(\lambda)$ are analytic in $\lambda \in \rho$. In fact, the analyticity follows from considering an analytic fundamental matrix solution Φ in $\lambda \in \rho$. Explicitly, the left-hand side of equation (4.66) is given by

$$\det_{\mathbb{C}^r}\big(\mathrm{id}_r + M(\lambda)\big) = 1 + \sum_{m=1}^{r} \frac{1}{m!} \sum_{i_1,\dots,i_m=1}^{r} \det_{\mathbb{C}^{i_m}} \begin{pmatrix} M_{i_1 i_1}(\lambda) & \cdots & M_{i_1 i_m}(\lambda) \\ \vdots & & \vdots \\ M_{i_m i_1}(\lambda) & \cdots & M_{i_m i_m}(\lambda) \end{pmatrix}. \tag{4.67}$$

Expanding the right-hand side of the above equation, substituting the Neumann series for the Jost solution Y^- and reordering the multiple integrals, it follows that

$$\det_{\mathbb{C}^r} D(\lambda) = 1 + \int_{\mathbb{R}} \mathrm{tr}_{\mathbb{C}^n}\left(Y_0^-(x) Z_0^+(x) V(x)\right) \mathrm{d}x + \sum_{j=2}^{\infty} \frac{1}{j!} \alpha_j^{(1)}(\lambda). \tag{4.68}$$

We can define $\mathcal{B}(\lambda)$ as an integral operator associated with $\alpha_j^{(1)}(\lambda)$ as coefficients of its regularised Fredholm determinant expansion (see Chapter 2). The existence of integral operator $\mathcal{B}(\lambda)$ is justified by the following arguments:

1. Since $M(\lambda)$ is finite rank operator and the set of finite rank operators is dense in $\mathfrak{I}_1$, there exists an operator $\mathcal{B}(\lambda) \in \mathfrak{I}_1$ such that $\|M(\lambda) - \mathcal{B}(\lambda)\|_{\mathfrak{I}_1} \leqslant \epsilon$. Hence, $\big|\det_{\mathbb{C}^r}(\mathrm{id}_r + M(\lambda)) - \det_1\big(\mathrm{id} + \mathcal{B}(\lambda)\big)\big| \leqslant \epsilon$ (for any two operators $\mathcal{K}_1, \mathcal{K}_2 \in \mathfrak{I}_1$, we have $|\det_1(\mathrm{id} - \mathcal{K}_1) - \det_1(\mathrm{id} - \mathcal{K}_2)| \leqslant \|\mathcal{K}_1 - \mathcal{K}_2\|_{\mathfrak{I}_1} \exp(1 + \|\mathcal{K}_1\|_{\mathfrak{I}_1} + \|\mathcal{K}_2\|_{\mathfrak{I}_1})$).

2. The determinant expansion in (4.67) with the Neumann series of the matrix-valued Jost solution Y^- substituted is similar to the determinant expansion of trace class operators (e.g. Plemelj–Smithies' formula (2.19) of Chapter 2). We note the similarity in the first two terms in the expansion (4.68), in particular the second term coincides with the integral trace of trace class operators (cf. (4.33)).

Note from (4.68) that the trace of $\mathcal{B}(\lambda)$ satisfies

$$\mathrm{tr}\, \mathcal{B}(\lambda) = \int_{\mathbb{R}} \mathrm{tr}_{\mathbb{C}^n}\left(\pm Y_0^{\pm}(x) Z_0^{\mp}(x) V(x)\right) \mathrm{d}x. \tag{4.69}$$

The minus sign in the right-hand side of (4.69) comes from using the other equivalent

definition of $D(\lambda)$, that is

$$D(\lambda) = \lim_{x\to-\infty} Z_0^-(x)Y^+(x).$$

Since both functions $\det_{\mathbb{C}^r} D(\lambda)$ and $\det_1\big(\mathrm{id} - \mathcal{K}(\lambda)\big)$ are analytic and vanish at eigenvalues of the operator $\mathcal{T}(\cdot)$ with equal multiplicity, they are equal, up to a non-vanishing analytic function. However, given that the first two terms (cf. (4.68)) in their series expansion are equal (e.g. (4.69) is equal to $\operatorname{tr}\mathcal{K}(\lambda)$ cf. (4.33)), it follows that

$$\det_{\mathbb{C}^r} D(\lambda) = \det_1\big(\mathrm{id} - \mathcal{K}(\lambda)\big).$$

Hence equation (4.65) follows from Theorem 4.3. □

Example 4.1 (KdV/mKdV equation [57, Theorem 3.1])**.** Consider the eigenvalue problem associated with the KdV/mKdV equation

$$-\frac{\mathrm{d}^3u}{\mathrm{d}x^3} + c\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}(\phi^q u) = \lambda u, \tag{4.70}$$

where $\phi^q(x) = \frac{1}{2}c(q+1)(q+2)\operatorname{sech}^2\big(\frac{1}{2}xq\sqrt{c}\big)$. For $\operatorname{Re}\lambda > 0$, the constant matrix $A_0(\lambda)$ associated with the first order system of (4.70) has 2 eigenvalues κ_j with $\operatorname{Re}\kappa_j > 0,\ (j = 2, 3)$, and one eigenvalue κ_1 with $\operatorname{Re}\kappa_1 < 0$. For $q = 1, 2$, the Evans function $E(\lambda)$ is given explicitly by

$$E(\lambda) = \left(\frac{\kappa_* + \sqrt{c}}{\kappa_* - \sqrt{c}}\right)^2, \tag{4.71}$$

where $\kappa_* = \min\{\operatorname{Re}\kappa_j,\ j = 1, 2, 3\}$. From Proposition 4.3, it follows that the integral operator $\mathcal{G}_1(\lambda)$ (cf. equations (4.44),(4.45)) associated with problem (4.70) is of trace class, for all $q \geqslant 1$. Hence considering the $(n-r)\times(n-r)$ matrix transmission coefficient $D(\lambda)$ $(n = 3, r = 2)$, we have, for all $q \geqslant 1$,

$$\begin{aligned}
\det_1\big(\mathrm{id} - \mathcal{K}(\lambda)\big) &= 1 - \int_{\mathbb{R}} Z_0^-(x)V(x)Y^+(x)\mathrm{d}x \\
&= 1 - \frac{\kappa_1}{(\kappa_1-\kappa_2)(\kappa_1-\kappa_3)}\int_{\mathbb{R}} \mathrm{e}^{-\kappa_1 x}\phi^q(x)u^+(x)\mathrm{d}x \\
&= \det_1\big(\mathrm{id} - \mathcal{G}_1(\lambda)\big).
\end{aligned}$$

In Figure 4.1, we display the Evans function $E(\lambda)$ and the Fredholm determinant $\det_1\big(\mathrm{id} - \mathcal{G}_1(\lambda)\big)$, for $q = 1$. Figure 4.1 indicates, for $q = 1, 2$, that that

$$\det_1\big(\mathrm{id} - \mathcal{G}_1(\lambda)\big) = \left(\frac{\kappa_* + \sqrt{c}}{\kappa_* - \sqrt{c}}\right)^2,$$

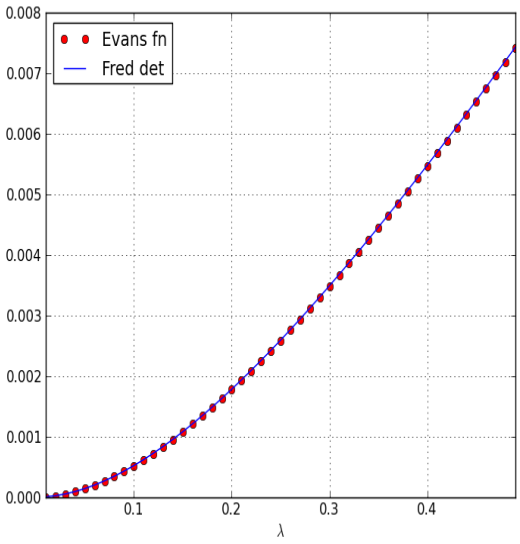

Figure 4.1: The Evans function given by (4.71) and the Fredholm determinant for $q = 1$ and $c = 1$.

Now we establish the connection between the Evans function and the determinant of the elliptic operator $\mathcal{T}(\lambda)$. Let $\det_\zeta$ denote the *zeta-regularised determinant* (cf. [59]). Then given an elliptic operator $\mathcal{A}$ with positive order and admitting a ray of minimal growth, its zeta-regularised determinant is given by (cf. [59])

$$\det_\zeta(\mathcal{A}) \coloneqq \exp\Big(-\frac{\partial}{\partial s}\zeta_{\mathcal{A}}(s)|_{s=0}\Big),$$

where

$$\zeta_{\mathcal{A}}(s) = \operatorname{tr}\mathcal{A}^{-s} = \sum_{\substack{\lambda_n \in \sigma_d(\mathcal{A}) \\ \lambda_n \neq 0}} \lambda_n^{-s}$$

with $\sigma_d(\mathcal{A})$ denoting the discrete spectrum of $\mathcal{A}$ and $\mathrm{Re}(s) \gg 0$. We remark that if

an elliptic operator $\mathcal{A}$ is Fredholm then we can define

$$\det_F(\mathcal{A}) \coloneqq \det_\zeta(\mathcal{A}). \tag{4.72}$$

From [50, Lemma 2.1], we know that the determinant of an elliptic operator given by $\mathcal{PQ}$, where $\mathcal{P}$ is elliptic operator and $\mathcal{Q}$ is Fredhlom operator of the form $\mathcal{Q} = \mathrm{id} + \mathcal{K}$ with $\mathcal{K}$ a trace class operator, satisfies the following relation

$$\det_\zeta(\mathcal{PQ}) = \det_\zeta(\mathcal{P}) \det_1(\mathrm{id} + \mathcal{K}). \tag{4.73}$$

Recall that $\mathcal{T}(\lambda) = \mathcal{T}_0(\lambda)\big(\mathrm{id} - \mathcal{K}_0(\lambda)V\big)$ and $\mathcal{T}_0(\lambda)$ are Fredholm, for all $\lambda \in \rho$. Then it follows from (4.72) and the above relation that

$$\begin{aligned} \det_F \mathcal{T}(\lambda) &= \det_F\Big(\mathcal{T}_0(\lambda)\big(\mathrm{id} - \mathcal{K}_0(\lambda)V\big)\Big) \\ &= \det_F \mathcal{T}_0(\lambda) \det_1\big(\mathrm{id} - \mathcal{K}_0(\lambda)V\big). \end{aligned} \tag{4.74}$$

Hence combining equation (4.74) and equation (4.62) connecting the Evans function with the determinant of $D(\lambda)$ in Theorem 4.3 yields

$$\frac{\det_F \mathcal{T}(\lambda)}{\det_F \mathcal{T}_0(\lambda)} = \frac{E(\lambda)}{c(\lambda)}. \tag{4.75}$$

Therefore

$$\det_F \mathcal{T}(\lambda) = \tilde{c}(\lambda) E(\lambda), \tag{4.76}$$

where $\tilde{c}(\lambda) = \det_F \mathcal{T}_0(\lambda)/c(\lambda)$. In particular if $\tilde{c}(\lambda) \equiv 1$, we have, for all $\lambda \in \rho,\ x_0 \in \mathbb{R}$,

$$\begin{aligned} \det_F \mathcal{T}_0(\lambda) &= \det_{\mathbb{C}^n} \Phi(x) \\ &= \exp\Big(\int_{x_0}^{x} \mathrm{tr}_{\mathbb{C}^n} A_0(y,\lambda)\mathrm{d}y\Big) \det_{\mathbb{C}^n} \Phi(x_0). \end{aligned}$$

In conclusion, the determinant of the Fredholm operator $\mathcal{T}(\lambda)$ or its zeta-regularised determinant reduces to the Evans function.

4.3.2 Hilbert–Schmidt operators

As seen in Subsection 4.1.1, the Birman–Schwinger operator $\mathcal{K}(\lambda)$, associated with the one dimensional travelling wave problems, is of Hilbert–Schmidt class for all $\lambda \in \rho$. Observe that Theorem 4.3 (connecting $\det_{\mathbb{C}^r} D(\lambda)$ and $E(\lambda)$) and Definition 4.2 (defining $D(\lambda)$ and (4.68), in particular) make sense independently of whether the operator $\mathcal{K}(\lambda)$ is of trace class or not. For some $\lambda \in \rho$ such that $\|\mathcal{K}(\lambda)\|_{\mathfrak{I}_2} < 1$, the Plemelj's formula for $\det_p$ (cf. Chapter 2) and in particular for $p = 2$ is given by

$$\det_2\Big(\mathrm{id} - \mathcal{K}(\lambda)\Big) = \exp\Big(\sum_{l=2}^{\infty} \frac{1}{l} \mathrm{tr}\, \mathcal{K}^l(\lambda)\Big).$$

Similarly, for some $\lambda \in \rho$ such that $\|\mathcal{B}(\lambda)\|_{\mathfrak{I}_1} < 1$, we have

$$\begin{aligned} \det_{\mathbb{C}^r} D(\lambda) &= \det_1\big(\mathrm{id} + \mathcal{B}(\lambda)\big) \\ &= \exp\Big(\sum_{l=1}^{\infty} \frac{1}{l} \mathrm{tr}\, \mathcal{B}^l(\lambda)\Big). \end{aligned} \tag{4.77}$$

From Theorem 4.4, if $\mathcal{K}(\lambda)$ is of trace class, we must have that $\mathrm{tr}\, \mathcal{K}^l(\lambda) = \mathrm{tr}\, \mathcal{B}^l(\lambda)$, for all $l \geqslant 1$. However if $\mathcal{K}(\lambda)$ is a Hilbert–Schmidt operator, then its trace might not be defined or might not be equal to $\mathrm{tr}\, \mathcal{B}(\lambda)$. Therefore $\mathrm{tr}\, \mathcal{K}^l(\lambda) = \mathrm{tr}\, \mathcal{B}^l(\lambda)$, for all $l \geqslant 2$. Hence using equation (4.77),

$$\det_{\mathbb{C}^r} D(\lambda) = \exp\big(\mathrm{tr}\, \mathcal{B}(\lambda)\big) \det_2\big(\mathrm{id} - \mathcal{K}(\lambda)\big), \tag{4.78}$$

where $\mathrm{tr}\, \mathcal{B}(\lambda)$ is defined in (4.69). Combining the above equation and equation (4.62) of Theorem 4.3, it follows that

$$\det_2\big(\mathrm{id} - \mathcal{K}(\lambda)\big) = \frac{E(\lambda)}{c(\lambda)} \exp\big(-\mathrm{tr}\, \mathcal{B}(\lambda)\big).$$

Consequently from equations (4.62) and (4.75),

$$\det_2\big(\mathrm{id} - \mathcal{K}(\lambda)\big) \exp\big(\mathrm{tr}\, \mathcal{B}(\lambda)\big) = \frac{\det_F \mathcal{T}(\lambda)}{\det_F \mathcal{T}_0(\lambda)}. \tag{4.79}$$

Note that the above relation extends the one given in (4.73) for trace class operators, i.e. $\mathcal{K}$ is Hilbert–Schmidt operator in $\mathcal{Q} = \mathrm{id} + \mathcal{K}$ given in (4.73).

Remark 4.11. Suppose that the perturbation V decays slowly so that it does not belong to L^1. Then the corresponding integral operator $\mathcal{K}(\lambda)$ is neither trace class nor Hilbert–Schmidt operator ($\|V\| \notin L^1$). However it is in $\mathfrak{I}_p$ for some $p \geqslant 3$. Following the same arguments which resulted in equation (4.78) and combining with equation (4.62), one establishes, for all $\lambda \in \rho$ and some $p \geqslant 3$, that

$$\det{}_p\big(\mathrm{id} - \mathcal{K}(\lambda)\big) = \frac{E(\lambda)}{c(\lambda)} \exp\Big(\sum_{l=1}^{p-1} \frac{(-1)^l}{l} \mathrm{tr}\, \mathcal{B}^l(\lambda)\Big).$$

Therefore relation similar to equation (4.79) follows, for some $p \geqslant 3$.

4.4 Regularised Fredholm determinants for fronts

In this section, we construct an integral operator associated with the p-regularised Fredholm determinants for the perturbation $\|V\|_{\mathbb{C}^{n\times n}} \notin L^1(\mathbb{R}, \mathbb{C})$. More often in our case, if $\sup_{x\in\mathbb{R}} \|V(x)\|_{\mathbb{C}^{n\times n}}$ is finite, then the travelling waves involved in the perturbation V are fronts. We focus on the case $A_0(x, \lambda) = A_0(\lambda)$ is constant and is analytic in $\lambda \in \mathbb{C}$, but the idea in this subsection can be extended to the x-dependent case. We also assume the following hypothesis.

Hypothesis 4.3. *Suppose that* $\lim_{x\to\pm\infty} V(x) = V^{\pm}$*, where* $V^+ \neq V^-$ *are constant-valued matrices, that*

$$\|V - V^{\pm}\|_{\mathbb{C}^{n\times n}} \in L^1(\mathbb{R}^{\pm}, \mathbb{C}).$$

Moreover, assume that eigenvalues of the matrices $A_0^{\pm}(\lambda) \coloneqq A_0(\lambda) + V^{\pm}$ *are semi-simple, for all* $\lambda \in \Lambda \subset \mathbb{C}$*, where* Λ *is the region introduced in Chapter 3.*

By $\kappa_j^{\pm} = \kappa_j^{\pm}(\lambda),\ j = 1, \ldots, r$, we denote the eigenvalues of $A_0^{\pm}(\lambda)$ with positive real parts and by $\tau_j^{\pm} = \tau_j^{\pm}(\lambda),\ j = r+1, \ldots, n$, the other eigenvalues with negative real parts, for all $\lambda \in \Lambda$. When $\lim_{x\to\pm\infty} V(x) = V^{\pm}$, the construction of the Green's function associated with the unperturbed problem $\mathcal{T}_0^{\pm}(\lambda) \coloneqq \mathrm{d}/\mathrm{d}x - A_0^{\pm}(\lambda)$ is not obvious as in Section 4.1. To circumvent this, we remark that it is possible to construct

a constant-coefficient differential operator defined, for all $\lambda \in \Lambda$, by

$$\widetilde{\mathcal{T}}_0(\lambda) \coloneqq \mathrm{d}/\mathrm{d}x - \widetilde{A}_0(\lambda), \tag{4.80}$$

where

$$P^{-1}(\lambda)\widetilde{A}_0(\lambda)P(\lambda) = \operatorname{diag}\left(\kappa_1^-, \ldots, \kappa_k^-, \tau_{k+1}^+, \ldots, \tau_n^+\right),$$

with

$$P(\lambda) = \begin{pmatrix} P^-(\lambda) & P^+(\lambda) \end{pmatrix}.$$

The columns of the matrices $P^{\pm}(\lambda)$ are the eigenvectors associated with eigenvalues τ_j^+ and κ_j^- respectively. If the eigenvalues of $A_0^{\pm}(\lambda)$ are simple, the matrix $P(\lambda)$ is given, for all $\lambda \in \Lambda$, by

$$P(\lambda) = \begin{pmatrix} 1 & \cdots & 1 & 1 & \cdots & 1 \\ \kappa_1^- & \cdots & \kappa_r^- & \tau_{r+1}^+ & \cdots & \tau_n^+ \\ \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\ (\kappa_1^-)^{n-1} & \cdots & (\kappa_r^-)^{n-1} & (\tau_{r+1}^+)^{n-1} & \cdots & (\tau_n^+)^{n-1} \end{pmatrix}.$$

Note that any nontrivial solution of $\mathcal{T}_0^{\pm}(\lambda)Y = 0$ satisfies $\widetilde{\mathcal{T}}_0(\lambda)Y = 0$ as well. And also choosing analytic eigenvectors of $A_0^{\pm}(\lambda)$, the constructed matrix $\widetilde{A}_0(\lambda)$ is analytic in $\lambda \in \Lambda$. Therefore, for all $\lambda \in \Lambda$, the differential operator $\widetilde{\mathcal{T}}_0(\lambda)$ is analytic in λ, and so is its corresponding resolvent operator $\widetilde{\mathcal{K}}_0(\lambda)$. The kernel of the resolvent operator $\widetilde{\mathcal{K}}_0(\lambda)$ is given by

$$\tilde{k}_0(x, y; \lambda) = \begin{cases} -\Phi(x, \lambda)Q\Phi^{-1}(y, \lambda), & x \leqslant y, \\ \Phi(x, \lambda)(\mathrm{id} - Q)\Phi^{-1}(y, \lambda), & y < x, \end{cases} \tag{4.81}$$

where Q is the projection operator onto the subspace decaying at $-\infty$ corresponding to the problem $\widetilde{\mathcal{T}}_0(\lambda)Y = 0$, and Φ is the fundamental matrix solution satisfying $\widetilde{\mathcal{T}}_0(\lambda)\Phi = 0$. The Birman–Schwinger operator corresponding to our new problem

$$\frac{\mathrm{d}}{\mathrm{d}x}Y = \left(\widetilde{A}_0(\lambda) + R(x)\right)Y \tag{4.82}$$

is given by

$$\widetilde{\mathcal{K}}(\lambda) = |R|^{1/2}\widetilde{\mathcal{K}}_0(\lambda)\widetilde{R},$$

where

$$R(x) = \begin{cases} V(x) - V^-, & x \leqslant 0 \\ V(x) - V^+, & x > 0, \end{cases} \tag{4.83}$$

and $\widetilde{R} = U|R|^{1/2}$ with U a partial isometry. Since $\widetilde{A}_0(\lambda)$ is constant-valued matrix and $\|R\|_{\mathbb{C}^{n\times n}} \in L^1$, it follows from Theorem 4.2 that the operator $\widetilde{\mathcal{K}}(\lambda)$ defined as above is of trace class, for all $\lambda \in \Lambda$. Given that the matrix-valued Jost solutions $Y^{\pm}$ of the original problem and that of the modified one $\widetilde{Y}^{\pm}$ corresponding to problem (4.82) are both exponentially bounded and their asymptotic limits coincide at $\pm\infty$, their column vectors are linearly dependent. Hence applying Theorem 4.4 for the modified problem (4.82), the Evans function $E(\lambda)$ of the original problem and the regularised Fredholm determinant associated with problem (4.82) satisfy the following equation

$$\begin{aligned} E(\lambda) &= \det_{\mathbb{C}^n}\begin{pmatrix} Y^- & Y^+ \end{pmatrix} \\ &= \tilde{c}(\lambda)\det_{\mathbb{C}^n}\begin{pmatrix} \widetilde{Y}^- & \widetilde{Y}^+ \end{pmatrix} \\ &= c(\lambda)\det_1\big(\mathrm{id} + \widetilde{\mathcal{K}}(\lambda)\big), \end{aligned} \tag{4.84}$$

where $\tilde{c}(\lambda)$ and $c(\lambda)$ are nonvanishing analytic functions. The analytic function $\tilde{c}(\lambda)$ is due to the linear dependence of the matrices $Y^{\pm}$ and $\widetilde{Y}^{\pm}$, and $c(\lambda)$ is the product of $c(\lambda)$ and the nonvanishing analytic function connecting the Evans function and Fredholm determinants of problem (4.82).

The subregion Λ when $V^- \neq V^+$ is given by (cf. [36, Lemma 2, p.138])

$$\Lambda = \mathbb{C} \setminus \big(\sigma_e^- \cup \sigma_e^+\big),$$

where $\sigma_e^{\pm}$ are the essential spectrum of $\mathcal{T}_0^{\pm}$ respectively.

Suppose that one considers the decomposition of the operator $\mathcal{T}$ given in (4.8) without taking into account the asymptotic limits of V. If for some $p \in \mathbb{N}$, the integral

operator $|V|^{1/2}\big(\mathrm{d}/\mathrm{d}x - A_0(\lambda)\big)^{-1}\widetilde{V} \in \mathfrak{I}_p$, then the zeros of its regularised Fredholm determinants might not coincide with eigenvalues of $\mathcal{T}(\lambda)$. This is because the domain in which $|V|^{1/2}\big(\mathrm{d}/\mathrm{d}x - A_0(\lambda)\big)^{-1}\widetilde{V}$ is defined, might is a subregion of, or contains, Λ given above. Therefore, this is one of the reasons why the construction of the Green's function is difficult for the case when $V^{\pm}$ are different. However, we have readily resolved this difficulty here.

Example 4.2. We consider the Fisher's equation written as a first order system of differential equations

$$\frac{\mathrm{d}}{\mathrm{d}x}Y = \begin{pmatrix} 0 & 1 \\ \lambda - 1 + 2\phi(x) & -c \end{pmatrix} Y,$$

where $\phi(x) = 1/\big(1 + \exp(x/\sqrt{6}\big)^{-2}$ and $c = 5/\sqrt{6}$ is the speed of the travelling wave solution. In this example, we apply our method for constructing the Fredholm determinant when the perturbation V satisfies Hypothesis 4.3. The perturbation

$$V = \begin{pmatrix} 0 & 0 \\ 2\phi & 0 \end{pmatrix}$$

is such that $\|V\|_{\mathbb{C}^{2\times 2}} \notin L^1$ and $\|V\|_{\mathbb{C}^{2\times 2}}$ is equal to 2 when x goes to $-\infty$ and 0 otherwise. We display the Fredholm determinant associated with the modified problem (4.82) without the nonvanishing function $c(\lambda)$ (only zeros of Fredholm determinants are important) and the Evans function $E(\lambda)$ corresponding to the original problem divided by $\det_{\mathbb{C}^n}(Y_0^- \quad Y_0^+)$, in Figure 4.2. It can be seen from Figure 4.2, that relation (4.84) holds with the nonvanishing analytic function $c(\lambda) \to 1$ as $\lambda \to \infty$. Numerically, our method presents an additional discontinuity in the kernel of the integral operator $\widetilde{\mathcal{K}}(\lambda)$ due to the discontinuity of the perturbation R in (4.83). Therefore, a suitable numerical method, which takes into account the discontinuity in the kernel function both on the diagonal and in the perturbation R, is required for best results.

4.5 Concluding remarks

We have shown in this chapter that for a class of travelling wave problems (those with constant-valued matrix $A_0(\lambda)$), the associated Birman–Schwinger operator is of trace class. Moreover, we have shown the connection between the Evans function

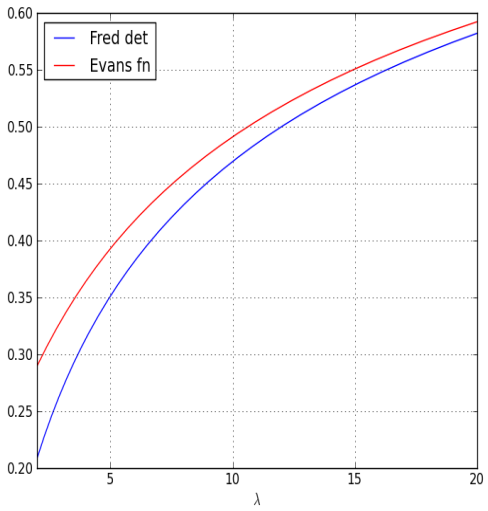

Figure 4.2: The Evans function of the original problem divided by $\det_{\mathbb{C}^n}(Y_0^- \quad Y_0^+)$ (red) and the Fredholm determinant for the modified problem (blue).

and modified Fredholm determinants through introducing the determinant of a finite dimensional determinant $D(\lambda)$ that we call the matrix transmission coefficients. Finally, we have constructed an appropriate integral operator in the case the matrix perturbation V is not in $L^1(\mathbb{R}, \mathbb{C}^{n\times n})$.

Chapter 5

Numerical evaluation of modified Fredholm determinants

5.1 Introduction

This chapter focuses on computing eigenvalues of integral operators in Hilbert space. To achieve this, numerical computation of p-modified Fredholm determinants (cf. [67] and [32]) is considered, since they locate eigenvalues of the corresponding integral operator, as well as their algebraic multiplicities (see [68], [32], [67], [34] and [11]).

Recently, the numerical evaluation of the Fredholm determinant was reintroduced by Bornemann in [10] for the purpose of computing distribution functions in random matrix theory. In particular, Bornemann generalised Hilbert's result to any quadrature rules which converge for continuous functions (Hilbert applied the rectangular rule to show the uniform convergence of the Fredholm determinant). In this chapter however, the uniform convergence is proved under a weaker assumption—the kernel is assumed to be integrable with respect to its second argument. Consequently, our uniform convergence result generalises that of Bornemann. Hence we extend the numerical evaluation of the Fredholm determinant to the p-modified Fredholm determinants. The difference between these two determinants is that the Fredholm determinant is associated with continuous kernels (the case studied by Bornemann) unlike the modified ones (our case), in the integral context. To prove our result, we use a result from collective compactness theory of Anselone [3]. Indeed we use the fact, that if the set

of finite rank operators approximating the integral operator is collectively compact, then the error converges uniformly in a totally bounded set. Consequently, the error in approximating eigenvalues of the integral operator, which is bounded by the error approximating the integral operator, converges uniformly (cf. [3], [5], [6] and [70]). This in turn yields uniform convergence of the p-modified Fredholm determinants.

From the numerical aspect, using the numerical method of Kang et al. [43] for solving integral equations, results in a uniform convergence in the resolvent set and exactness in the spectrum. Indeed, this suggests that computing the determinant is nothing other than an interpolation in which the zeros are the interpolation points. From this point of view, the convergence result is confirmed, since from interpolation theory, uniform convergence is guaranteed for any continuous function in a bounded domain. To compute the infinite determinants numerically, the integral equation is approximated by a system of algebraic equations whose determinant is then computed. Furthermore, the computation of higher order determinants is demonstrated, in particular for $p = 3, 4$.

5.2 Convergence analysis

Let $[a, b]$ be a finite interval of $\mathbb{R}$, and let $C\big([a, b]\big)$ be the space of continuous functions on $[a, b]$, equipped with the uniform norm $\|\cdot\|_\infty$. For all $z \in \mathbb{C}$ and $u \in C\big([a, b]\big)$, the eigenvalue problem reads

$$(\mathrm{id} + z\mathcal{K})u = 0, \tag{5.1}$$

where, for all $x \in (a, b)$,

$$\mathcal{K}u(x) = \int_a^b k(x, y)u(y)\mathrm{d}y \tag{5.2}$$

with $k(x, y)$ a measurable function.

In this section, we prove uniform convergence of the modified/regularised Fredholm determinants for bounded $z \in \mathbb{C}$. As a result, we give the rate of convergence in the spectrum and in the resolvent set of $\mathcal{K}$. Moreover, we demonstrate how to compute the modified/regularised Fredholm determinants numerically.

To solve problem (5.1), two methods are generally used: the expansion or projection, and the quadrature methods (Nyström-type). Here we focus on the latter method. However, the results in this chapter are also applicable for the projection methods, under the hypotheses stated in [70]. These hypotheses roughly assume that $\mathcal{K}$ is compact and that both $\|\mathcal{K}-P_N\mathcal{K}\|$ and $\|\mathcal{K}_N-P_N\mathcal{K}\|$ tend to zero as $N\to\infty$, where P_N is a projection operator and $\mathcal{K}_N$ is an approximation of $\mathcal{K}$. The type of kernel functions $k(x,y)$ that we shall consider are continuous everywhere in the domain except on the diagonal, i.e., the set $\{(x,y)\in[a,b]\times[a,b]\colon x=y\}$, and they also satisfy the following hypotheses.

Hypothesis 5.1. *Assume that for all* $x\in[a,b]$, $k(x,\cdot)\in L^1\big([a,b]\big)$,

$$\sup_{x\in[a,b]}\int_a^b |k(x,y)|\mathrm{d}y<\infty, \tag{5.3}$$

and for $x_1,x_2\in[a,b]$

$$\int_a^b \big|k(x_1,y)-k(x_2,y)\big|\mathrm{d}y\to 0,\ \ as\ x_1\to x_2. \tag{5.4}$$

Any integral operator $\mathcal{K}$ associated with problem (5.1) and with kernel $k(x,y)$ satisfying the above hypothesis maps $C\big([a,b]\big)$ into itself, and is compact. Indeed for all $x_1,x_2\in[a,b]$ and $u\in C\big([a,b]\big)$, we have

$$|\mathcal{K}u(x_1)-\mathcal{K}u(x_2)|\leqslant\|u\|_\infty\int_a^b\big|k(x_1,y)-k(x_2,y)\big|\mathrm{d}y. \tag{5.5}$$

As x_1 goes to x_2, and using (5.4), it follows that the integral operator $\mathcal{K}$ maps $C\big([a,b]\big)$ the space of continuous functions into itself. Let

$$S=\{u\in C\big([a,b]\big)\colon\|u\|_\infty\leqslant 1\}. \tag{5.6}$$

To show the compactness of $\mathcal{K}$, we need to show that the set $\mathcal{K}(S)$ is totally bounded in $C(a,b)$. This is equivalent to showing that $\mathcal{K}(S)$ is bounded and equicontinuous in $C\big([a,b]\big)$ (Arzelà–Ascoli theorem). The boundedness of $\mathcal{K}(S)$ follows directly from (5.3), i.e. for all $u\in S$,

$$\|\mathcal{K}u\|<\infty$$

since for all $x \in [a,b]$ and $u \in S$

$$|\mathcal{K}u(x)| \leqslant \sup_{x\in[a,b]} \int_a^b |k(x,y)|\mathrm{d}y.$$

For all $u \in S$ and $x_1, x_2 \in [a,b]$, the equicontinuity of $\mathcal{K}(S)$ follows from taking the limit as x_1 goes to x_2 in equation (5.5) and invoking (5.4). Consequently we have that the operator $\mathcal{K}$ is compact.

Henceforth, we shall assume that the kernel function k satisfying Hypothesis 5.1 is given by

$$k = g \times h, \tag{5.7}$$

where g satisfies Hypothesis 5.1 and h is continuous everywhere in the domain. Note that with Hypothesis 5.1, we can consider $g(x,y) = |x-y|^{-\alpha}$ with $0 \leqslant \alpha < 1$ since the corresponding integral operator is compact. Assume for all $x \in [a,b]$, $u \in C\big([a,b]\big)$ and for sufficiently large N that

$$\|h(x,\cdot)u(\cdot) - \sum_{j=1}^{N} h_j(x)u(y_j)P_j(\cdot)\|_\infty \to 0, \tag{5.8}$$

where the P_j is a polynomial interpolation of order j in $C\big([a,b]\big)$, y_j are the nodal points in $[a,b]$ and $h_j(x) = h(x,y_j)$. Then we define the operator $\mathcal{K}_N$ by

$$\mathcal{K}_N u(x) = \sum_{j=1}^{N} w_j(x)h_j(x)u(y_j), \tag{5.9}$$

where for fixed $x \in [a,b]$ and $j = 1,\ldots,N$

$$w_j(x) = \int_a^b g(x,y)P_j(y)\mathrm{d}y.$$

Under Hypothesis 5.1, the operator $\mathcal{K}_N$ maps $C\big([a,b]\big)$ to itself. Indeed, note that the continuity of w_j follows directly from the assumption on the function g. Therefore, it follows from the continuity assumption of h that the product $w_j(x)h_j(x)$ is continuous for all $x \in [a,b]$. For $N \geqslant 1$, $x \in [a,b]$, there exists a constant $c_N > 0$ such that for

all $u \in S$ (i.e. $\|u\|_\infty \leqslant 1$), we have

$$\begin{aligned}\big|\mathcal{K}_N u(x)\big| &\leqslant \sum_{j=1}^{N} \big|w_j(x)h_j(x)\big| \\ &\leqslant \sup_{x\in[a,b]} \sum_{j=1}^{N} \big|w_j(x)h_j(x)\big| \\ &\leqslant c_N \|h_j\|_\infty \sup_{x\in[a,b]} \int_a^b |g(x,y)|\mathrm{d}y < \infty. \end{aligned} \tag{5.10}$$

The last estimate implies that $\mathcal{K}_N u$ is bounded in $C\big([a,b]\big)$, for $N \geqslant 1$. Moreover, we have that $\mathcal{K}_N$ is compact since it is finite rank operator, as $\dim(\operatorname{ran}\mathcal{K}_N) \leqslant N$. In conclusion, the operator $\mathcal{K}_N$ maps $C\big([a,b]\big)$ to itself, and is compact.

Remark 5.1. Alternatively for fixed $x \in [a,b]$, we can approximate $h(x,y)u(y)$ with some orthogonal polynomial basis in L^2 in equation (5.8). This method is also used in Section 5.3.

Given the operator $\mathcal{K}_N$, equation (5.1) is replaced, for all $x \in [a,b]$, by

$$u_N(x) = -z \sum_{j=1}^{N} w_j(x)h_j(x)u_N(y_j). \tag{5.11}$$

Applying the Nyström method (cf. [55]) in the above equation, i.e., substituting $x = y_i$ in equation (5.11), yields a finite dimensional eigenvalue problem given by

$$u_N(y_i) = -z \sum_{j=1}^{N} w_j(y_i)h_j(y_i)u_N(y_j),\ i = 1,\dots,N. \tag{5.12}$$

Note that the two equations (5.11) and (5.12) are equivalent. That is, if $u_N(x)$ satisfies (5.11) then it also satisfies (5.12) when $x = y_i$. Conversely, if $u_N(y_i)$ satisfies (5.12) then $u_N(x)$ is uniquely determined by its values at the node points $\{y_i\}$ in (5.11).

To illustrate the use of Fredholm determinants, suppose that the kernel k is continuous and that the associated integral operator $\mathcal{K}$ is approximated by a Gaussian quadrature in $[a,b]$ (any Gaussian quadrature for finite domain is valid, e.g. Chebyshev, Legendre). Then for all $x \in [a,b]$ and $j = 1,\dots,N$, the quadrature weights

$w_j(x) = w_j$ are constant in (5.11), and $k = h$ in the product defining the kernel k from (5.7), i.e. $g \equiv 1$. From equation (5.12), one can then deduce that eigenvalues of $\mathcal{K}_N$ are precisely the zeros of the function $d_N(z)$ defined by

$$d_N(z) = \det_{\mathbb{C}^N}(\mathrm{id}_N + zA), \tag{5.13}$$

where $A = \big((w_j k(y_i, y_j)\big)_{i,j=1}^{N}$. Given that the kernel k is continuous everywhere in the domain, then for bounded $z \in \mathbb{C}$, the determinant $d_N(z)$ converges uniformly to the Fredholm determinant $d(z)$ defined in (2.4) (cf. [10, Theorem 6.1]).

Remark 5.2. Implicitly, the collective compactness of the set of operators $\{\mathcal{K}_N\}_{N\geqslant 1}$ (see Definition 5.1 below) is used in Theorem 6.1 of [10], since the continuity of the kernel k and the application of a Gaussian quadrature to approximate the integral operator are the guaranteeing sufficient conditions (cf. [3]).

Let $\mathbb{B}$ denote the set of bounded linear operators on $C\big([a,b]\big)$. To generalise Theorem 6.1 in [10] to any integral operator $\mathcal{K} \in \mathfrak{I}_p$ with kernel given by (5.7) and g satisfying Hypothesis 5.1, we shall need the following definition:

Definition 5.1 (Collectively compact, Anselone [3])**.** A set of operators $\{\mathcal{K}_n\}_{n\geq 1} \subset \mathbb{B}$ is called *collectively compact* if

A. $\mathcal{K}$ and $\mathcal{K}_n$ are linear operators on the Banach space B into itself.

B. $\mathcal{K}_n u \to \mathcal{K}u$ as $n \to \infty$, for all $u \in B$ and $n \geqslant 1$.

C. The set $\{\mathcal{K}_n u : \ n \geqslant 1, \ \|u\| \leqslant 1\}$ has compact closure in B.

Definition 5.2 (Anselone [3])**.** A set of operators $\mathcal{A} \subset \mathbb{B}$ is collectively compact, if the set

$$\mathcal{A}(S) = \{\mathcal{K}u : \ \mathcal{K} \in \mathcal{A}, \ u \in S\},$$

where S is given for example by (5.6), is relatively compact (relatively compact, sequentially compact and totally bounded are equivalent in a complete space [3]). A sequence of operators in $\mathbb{B}$ is collectively compact whenever the corresponding set is.

In what follows, c is always a positive constant. Under Hypothesis 5.1, we show that the set of operators $\{\mathcal{K}_N\}_{N\geqslant 1}$ defined in (5.9) is collectively compact. Indeed, the

operator $\mathcal{K}_N$ satisfies A. Regarding B, observe that for all $x \in [a,b]$ and $u \in C\big([a,b]\big)$,

$$|\mathcal{K}u(x) - \mathcal{K}_N u(x)| \leqslant c \sup_{x\in[a,b]} \int_a^b \big|h(x,y)u(y) - [h(x,y)u(y)]_N\big| \mathrm{d}y$$

$$= c \sup_{x\in[a,b]} \|h(x,\cdot)u - [h(x,\cdot)u]_N\|_{L^1},$$

where $[h(x,y)u(y)]_N$ approximates $h(x,y)u(y)$, i.e. it is given by the right-hand side of (5.8). For all $x, y \in [a,b]$ since the function $h(x,y)u(y)$ is continuous, it follows from interpolation theory that the right-hand side of the above inequality converges to zero as N goes to infinity. Hence for large N,

$$\mathcal{K}_N u \to \mathcal{K}u. \tag{5.14}$$

To show condition C, we again use the Arzelà–Ascoli theorem. Given the above pointwise convergence (5.14), the set of operators $\{\mathcal{K}_N\}_{N\geqslant 1}$ is uniformly bounded [3], i.e., for all $N \geqslant 1$ there exists a positive constant c (different from the previous one) such that

$$\|\mathcal{K}_N\| \leqslant c.$$

Therefore the set $\{\mathcal{K}_N(S)\}_{N\geqslant 1}$ is uniformly bounded as well. For all $x_1, x_2 \in [a,b]$, observe that

$$\begin{aligned}
|\mathcal{K}_N u(x_1) - \mathcal{K}_N u(x_2)| &\leqslant \sum_{j=1}^{N} |w_j(x_1)h_j(x_1) - w_j(x_2)h_j(x_2)| \\
&\leqslant \sum_{j=1}^{N} \Big(|(w_j(x_1) - w_j(x_2))h_j(x_1)| \\
&\qquad + \big|(h_j(x_1) - h_j(x_2))w_j(x_2)\big| \Big) \\
&\leqslant \sum_{j=1}^{N} \Big(\|h_j\| \ \big|w_j(x_1) - w_j(x_2)\big| \\
&\qquad + \|w_j\| \ \big|h_j(x_1) - h_j(x_2)\big| \Big).
\end{aligned}$$

Since the functions w_j and h_j are continuous for all $y_j \in [a,b]$, it follows that for all

$N \geqslant 1$ and as x_1 goes to x_2,

$$|\mathcal{K}_N u(x_1) - \mathcal{K}_N u(x_2)| \to 0.$$

Hence the equicontinuity is established. By Arzelà–Ascoli theorem, the set of functions $\{\mathcal{K}_N(S)\}_{N\geqslant 1}$ has a compact closure, and so by Definition 5.2 we have that the set of operators $\{\mathcal{K}_N\}_{N\geqslant 1}$ is collectively compact.

Having proved the compactness property of the operators $\mathcal{K}$ and $\{\mathcal{K}_N\}_{N\geqslant 1}$, we are now ready to show the uniform convergence result for integral operator $\mathcal{K} \in \mathfrak{I}_p$ for $p \geqslant 1$. The outline of our proof is as follows: assume that the set of operators $\{\mathcal{K}_N\}_{N\geqslant 1}$, obtained either by quadrature or by projection methods, is collectively compact. Then an eigenvalue λ of $\mathcal{K}$ is the limit of a sequence of eigenvalues λ_N of $\mathcal{K}_N$ (cf. [5,70]). It follows that the nth power of λ is also the limit of the nth power of λ_N. Consequently, for bounded $z \in \mathbb{C}$, one gets uniform convergence in approximating the p-modified Fredholm determinants. This is because the error in approximating the p-modified Fredholm determinants depends on the error approximating eigenvalue, λ of $\mathcal{K}$, which is in turn bounded uniformly by $\mathcal{K}u - \mathcal{K}_N u$. In brief, the uniform convergence of the eigenvalues implies the uniform convergence of the p-modified Fredholm determinants.

Remark 5.3. There exist integral operators, $\mathcal{K}$ that do not fully satisfy Hypothesis 5.1 but are compact. The integral kernel of such operators are given, for example, by $h(x,y)|x-y|^{-\alpha}$ where $h(x,y)$ is assumed to be continuous and $\alpha > 1$. In particular for $\alpha = 3/2$, the integral operator $\mathcal{K} \in \mathfrak{I}_4$ (cf. [11]). In that case, the convergence analysis of this chapter no longer applies since $w_j(x)$ is not Lebesgue integrable. However, as long as one is interested in eigenvalues, one strategy that could be used is to compute the Fredholm determinant of the nth power of the operator $\mathcal{K}$, since for some $n \in \mathbb{N}$, the nth power integral operator $\mathcal{K}^n$ is of trace class and its kernel is continuous. From this, a relation between the Fredholm determinant corresponding to $\mathcal{K}^n$ and the p-modified Fredholm determinants associated with $\mathcal{K}$, is established. Therefore one deduces the p-modified Fredholm determinants associated with $\mathcal{K}$ from the Fredholm determinant associated with $\mathcal{K}^n$ (cf. Theorem 5.1 and Remark 5.4).

Theorem 5.1. *Suppose that* $\mathcal{K} \in \mathfrak{I}_2$*, then*

$$\det_1(\mathrm{id} - z^2\mathcal{K}^2) = \det_2(\mathrm{id} - z\mathcal{K}) \det_2(\mathrm{id} + z\mathcal{K}).$$

Moreover, if $\det_2(\mathrm{id} - z\mathcal{K}) = \det_2(\mathrm{id} + z\mathcal{K})$ *then*

$$(\det_2(\mathrm{id} - z\mathcal{K}))^2 = \det_1(\mathrm{id} - z^2\mathcal{K}^2).$$

If $\mathcal{K} \in \mathfrak{I}_3$ *then* $\mathcal{K}^2 \in \mathfrak{I}_2$ *and we have*

$$\det_2(\mathrm{id} - z^2\mathcal{K}^2) = \det_3(\mathrm{id} - z\mathcal{K}) \det_3(\mathrm{id} + z\mathcal{K}).$$

Proof. Since the product of two Hilbert–Schmidt operators is of trace class, we have

$$\begin{aligned}
\det_1(\mathrm{id} - z^2\mathcal{K}^2) &= \prod_{n=1}^{\infty}(1 - z^2\lambda_n^2) \\
&= \prod_{n=1}^{\infty}\Big[(1 - z\lambda_n)\exp(\lambda_n z)(1 + z\lambda_n)\exp(-\lambda_n z)\Big] \\
&= \prod_{n=1}^{\infty}\Big[(1 - z\lambda_n)\exp(\lambda_n z)\Big] \prod_{n=1}^{\infty}\Big[(1 + z\lambda_n)\exp(-\lambda_n z)\Big] \\
&= \det_2(\mathrm{id} - z\mathcal{K}) \det_2(\mathrm{id} + z\mathcal{K})
\end{aligned}$$

Now if $\mathcal{K} \in \mathfrak{I}_3$ then observe that $\mathcal{K}^2$ satisfies (cf. [32, Theorem 11.2, Chap IV])

$$\mathrm{tr}\,|\mathcal{K}^2|^2 \leqslant (\mathrm{tr}\,|\mathcal{K}|^4)^{1/2} \leqslant (\mathrm{tr}\,|\mathcal{K}|^3)^{2/3} < \infty. \tag{5.15}$$

Hence $\mathcal{K}^2$ is Hilbert–Schmidt. It then follows that

$$\begin{aligned}\det_2(\mathrm{id} - z^2\mathcal{K}^2) &= \prod_{n=1}^{\infty}(1 - z^2\lambda_n^2)\exp(z^2\lambda_n^2) \\ &= \prod_{n=1}^{\infty}\Big((1 - z\lambda_n)\exp(\lambda_n z + z^2\lambda_n^2/2) \\ &\qquad \times (1 + z\lambda_n)\exp(-\lambda_n z + z^2\lambda_n^2/2)\Big) \qquad (5.16) \\ &= \det_3(\mathrm{id} - z\mathcal{K})\det_3(\mathrm{id} + z\mathcal{K}).\end{aligned}$$

□

The inequalities (5.15) are obtained by combining the following inequalities

$$\mathrm{tr}\,|\mathcal{K}^2|^2 \leqslant (\mathrm{tr}\,|\mathcal{K}|^3)^{2/3},\ \mathrm{tr}\,|\mathcal{K}^2|^2 \leqslant (\mathrm{tr}\,|\mathcal{K}|^4)^{1/2} \text{ and } (\mathrm{tr}\,|\mathcal{K}^2|^4)^{1/4} \leqslant (\mathrm{tr}\,|\mathcal{K}|^3)^{1/3}.$$

Remark 5.4. If $\mathcal{K} \in \mathfrak{I}_4$ then $\mathcal{K}^2 \in \mathfrak{I}_2$ (cf. $\mathrm{tr}\,|\mathcal{K}^2|^2 \leqslant (\mathrm{tr}\,|\mathcal{K}|^4)^{1/2} < \infty$). Indeed we have

$$\det_2(\mathrm{id} - z^2\mathcal{K}^2) = \det_4(\mathrm{id} - z\mathcal{K})\det_4(\mathrm{id} + z\mathcal{K}).$$

The proof is as above, we replace (5.16) by

$$\det_4(\mathrm{id} \pm z\mathcal{K}) = \prod_{n=1}^{\infty}(1 \pm z\lambda_n)\exp(\mp\lambda_n z + z^2\lambda_n^2/2 \mp z^3\lambda_n^3/3).$$

In what follows, we set for all $p \geqslant 1$ and $z \in \mathbb{C}$,

$$d_p(z) \coloneqq \det_p(\mathrm{id} + z\mathcal{K}) \quad \text{and} \quad d_{Np}(z) \coloneqq \sum_{k=0}^{\infty}\alpha_{(kN)}^{(p)}z^k/k!.$$

where $\alpha_{(kN)}^{(p)}$ are defined by (2.20) and (2.21) with $\mathrm{tr}\,\mathcal{K}_N$ substituted by $\mathrm{tr}\,\mathcal{K}$.

Remark 5.5. 1. Note that the function $d_{Np}(z)$ is equal to the finite dimensional determinant associated with the matrix $A = \big((w_j(y_i)h(y_i, y_j)\big)_{i,j=1}^N$, i.e.

$$d_{Np}(z) = \det_{\mathbb{C}^N}(\mathrm{id}_N + zA). \qquad (5.17)$$

2. As mentioned in Bornemann [10] and proved in Meyer [54, p. 492], the series defining the finite dimensional determinant $d_{Np}(z)$ must stop at $n = N$, since it is a polynomial of degree at most N.

3. Since $\mathcal{K}_N$ is a finite rank operator and equations (5.11) and (5.12) are equivalent, then $\operatorname{tr} \mathcal{K}_N = \operatorname{tr}_{\mathbb{C}^N} A$.

Theorem 5.2. *Assume that $\mathcal{K}$ given in* (5.7) *is in $\mathfrak{I}_p$, and $\{\mathcal{K}_N\}_{N\geqslant 1}$ is collectively compact with $\mathcal{K}_N$ defined by* (5.9)*. Then for $p \geqslant 1$, we have*

$$d_{Np}(z) \to d_p(z)$$

converges uniformly for all bounded z as $N \to \infty$.

Proof. Let $z \in \mathbb{C}$ be bounded by $M > 0$. Then

$$|d_p(z) - d_{Np}(z)| \leqslant \sum_{j=0}^{\infty} |\alpha_j^{(p)} - \alpha_{(jN)}^{(p)}| \; M^j/j!. \tag{5.18}$$

Observe from (2.21) and (2.22) that

$$\begin{aligned}
|\alpha_j^{(p)} - \alpha_{(jN)}^{(p)}| &\leqslant \sum_{l=1}^{j} |\alpha_{j-l}^{(p)} \nu_l^{(p)} - \alpha_{((j-l)N)}^{(p)} \nu_{(lN)}^{(p)}| \\
&\leqslant \sum_{l=1}^{j} \left(|\alpha_{j-l}^{(p)} - \alpha_{((j-l)N)}^{(p)}| \; |\nu_l^{(p)}| + |\nu_l^{(p)} - \nu_{(lN)}^{(p)}| \; |\alpha_{((j-l)N)}^{(p)}| \right) \\
&\leqslant \sum_{l=1}^{j} c_l |\nu_l^{(p)} - \nu_{(lN)}^{(p)}| \\
&\leqslant c \sum_{l=1}^{j} \left| \nu_l^{(p)} - \nu_{(lN)}^{(p)} \right|,
\end{aligned} \tag{5.19}$$

where c_l are positive coefficients and $c = \max_{l=1,\ldots,j}\{c_l\}$. For all $j \geqslant p$,

$|\nu_l^{(p)} - \nu_{(lN)}^{(p)}| = |\operatorname{tr}\mathcal{K}^l - \operatorname{tr}\mathcal{K}_N^l|$. Therefore

$$\begin{aligned}|\operatorname{tr}\mathcal{K}^l - \operatorname{tr}\mathcal{K}_N^l| &= \Big|\sum_{n=1}^{\infty}\lambda_n^l - \sum_{n=1}^{N}\lambda_{(nN)}^l\Big| \\ &\leqslant \Big|\sum_{n=1}^{N}\lambda_n^l - \sum_{n=1}^{N}\lambda_{(nN)}^l\Big| + \Big|\sum_{n=N+1}^{\infty}\lambda_n^l\Big|,\end{aligned}$$

where λ_n and λ_{nN} are eigenvalues of the operators $\mathcal{K}$ and $\mathcal{K}_N$ respectively.
As N goes to infinity,

$$\sum_{n=N+1}^{\infty}|\lambda_n|^l \to 0.$$

Hence

$$\Big|\sum_{n=N+1}^{\infty}\lambda_n^l\Big| \leqslant \sum_{n=N+1}^{\infty}\big|\lambda_n\big|^l \to 0.$$

Given that $\{\mathcal{K}_N\}_{N\geqslant 1}$ is collectively compact, for sufficiently large N, $\epsilon > 0$ and for $n \in \{1,\ldots,N\}$ (cf. [5] and [70] and [3, Theorem 4.8])

$$|\lambda_n - \lambda_{(nN)}| \leqslant \epsilon.$$

Hence it follows that

$$\begin{aligned}|\lambda_n^l - \lambda_{(nN)}^l| &= \big|\lambda_n - \lambda_{(nN)}\big|\Big|\sum_{m=0}^{l-1}\lambda_n^m\lambda_{(nN)}^{l-m}\Big| \\ &\leqslant \big|\lambda_n - \lambda_{(nN)}\big|\sum_{m=0}^{l-1}\big|\lambda_n^m\lambda_{(nN)}^{l-m}\big| \qquad (5.20)\\ &\leqslant l\big|\lambda_n\big|^l\epsilon. \qquad (5.21)\end{aligned}$$

Since for sufficiently large N,

$$\sum_{m=0}^{l-1}\lambda_n^m\lambda_{(nN)}^{l-m} \approx l|\lambda_n|^l. \qquad (5.22)$$

From inequality (5.21) and the continuous embedding of $\mathfrak{I}_p \subset \mathfrak{I}_q$ for $p < q$ (cf (2.17)

of Chapter 2), we have

$$\sum_{n=1}^{N}\left|\lambda_n^l - \lambda_{(nN)}^l\right| \leqslant \epsilon l \sum_{n=1}^{N}\left|\lambda_n\right|^l \leqslant \epsilon l \|\mathcal{K}\|_{\mathfrak{I}_p}^p.$$

Thus for N large enough and ϵ chosen arbitrarily small,

$$|\operatorname{tr}\mathcal{K}^l - \operatorname{tr}\mathcal{K}_N^l| \leqslant \epsilon. \tag{5.23}$$

Consequently combining (5.23), (5.19) and (5.18),

$$|d_p(z) - d_{Np}(z)| \leqslant \epsilon \quad \text{as} \quad N \to \infty.$$

□

Under the assumption that the set of operators $\{\mathcal{K}_N\}_{N\geqslant 1}$ is collectively compact and exploiting the results of [6], [5] and [70], we now estimate the rate of convergence in evaluating the determinant $d_{Np}(z)$ at the spectrum of $\mathcal{K}$, $\sigma_d(\mathcal{K})$.

Theorem 5.3. *Assume that $\mathcal{K}$ and $\{\mathcal{K}_N\}_{N\geqslant 1}$ are given as in Theorem 5.2. Let $n_0 < N$ be fixed and $\lambda_{n_0} \neq 0$ and $\lambda_{n_0 N}$ denote the eigenvalues of $\mathcal{K} \in \mathfrak{I}_p$ and $\mathcal{K}_N$, respectively. Then for some N sufficiently large and for $p \geqslant 1$, we have*

$$|d_p(z_{n_0}) - d_{Np}(z_{n_0})| \leqslant c \max_{1\leqslant i\leqslant m}\{\|\mathcal{K}u_i - \mathcal{K}_N u_i\|^{1/\nu}\}, \tag{5.24}$$

where $z_{n_0} = \lambda_{n_0}^{-1}$, $\{u_1, \cdots, u_m\}$ is a basis for $\operatorname{Ker}(\mathcal{K} - \lambda_{n_0}\mathrm{id})^\nu$ and m and ν are the multiplicity and the index[2] of λ_{n_0}, respectively.

Proof. For simplicity, we consider the case $p = 1$. However the proof holds for $p \geqslant 2$ by using a finite dimensional version of p-modified Fredholm determinants in (2.23) of Chapter 2. Evaluating the Fredholm determinant at its zero $z_{n_0} = \lambda_{n_0}^{-1}$, for fixed

[2]The smallest positive integer l such that $\operatorname{Ker}(\mathcal{K} - \lambda_{n_0}\mathrm{id})^l = \operatorname{Ker}(\mathcal{K} - \lambda_{n_0}\mathrm{id})^{l+1}$

$n_0 < N$ and $\lambda_{n_0} \neq 0$, we have

$$\begin{aligned} |d(z_{n_0}) - d_N(z_{n_0})| &= |d_N(z_{n_0})| \\ &= \Big|\prod_{n=1}^{N}(1 - \lambda_{n_0}^{-1}\lambda_{(nN)})\Big| \\ &= \Big|\prod_{n=1}^{N}\left[\lambda_{n_0}^{-1}\left(\lambda_{n_0} - \lambda_{(nN)}\right)\right]\Big| \\ &= |\lambda_{n_0}|^{-N}\prod_{n=1}^{N}|\lambda_{n_0} - \lambda_{(nN)}|. \end{aligned} \tag{5.25}$$

Since the set of operators $\{\mathcal{K}_N\}_{N\geqslant 1}$ is collectively compact, it follows from [6] and [70, Theorem 3] when $n = n_0$ in the right-hand side of (5.25), for sufficiently large N, that

$$|d(z_{n_0}) - d_N(z_{n_0})| \leqslant c \max_{1\leqslant i\leqslant m}\{\|\mathcal{K}u_i - \mathcal{K}_N u_i\|^{1/\nu}\}.$$

□

Pointwise convergence implies uniform convergence in a totally bounded set [3, Proposition 1.7]. Therefore, since the set $\{\mathcal{K}_N(S)\}_{N\geqslant 1}$ is totally bounded, $\mathcal{K}_N u_i$ converges uniformly to $\mathcal{K}u_i$ as $N \to \infty$, i.e.

$$\|\mathcal{K}u_i - \mathcal{K}_N u_i\| \to 0 \text{ as } N \to \infty.$$

For the projection method, it suffices to replace the right-hand side of (5.24) by the error bound in [70, Theorem 3].

Theorem 5.4. *Assume that $\mathcal{K}$ and $\{\mathcal{K}_N\}_{N\geqslant 1}$ are given as in Theorem 5.3. Then for some sufficiently large N and z an element of the resolvent set $\rho(\mathcal{K})$, we have*

$$|d_p(z) - d_{Np}(z)| \leqslant c\beta(N, \nu_{n_0})\|\mathcal{K}\|_{\mathfrak{I}_p}^p, \tag{5.26}$$

where

$$\beta(N, \nu_{n_0}) = \max_{1\leqslant i\leqslant m_{n_0}}\{\|\mathcal{K}u_i - \mathcal{K}_N u_i\|^{1/\nu_{n_0}}\} \tag{5.27}$$

and $\nu_{n_0} = \max\limits_{n=1,\ldots,N}\{\nu_n\}$ with ν_n are the indices of the eigenvalues λ_n.

Proof. Suppose that $z \in \rho(\mathcal{K})$. Then combining equation (5.20) and (5.22), and the error estimate of [6] for each $\lambda_n,\ n = 1, \cdots, N$, we have for all $k \geqslant p$ and for some sufficiently large N,

$$|\operatorname{tr} \mathcal{K}^k - \operatorname{tr} \mathcal{K}_N^k| \leqslant ck \sum_{n=1}^{N} |\lambda_n|^k \max_{1 \leqslant i \leqslant m_n} \{\|\mathcal{K}u_i - \mathcal{K}_N u_i\|^{1/\nu_n}\}.$$

Given ν_{n_0} then for all $n = 1, \ldots, N$,

$$\max_{1 \leqslant i \leqslant m_n} \{\|\mathcal{K}u_i - \mathcal{K}_N u_i\|^{1/\nu_n}\} \leqslant \beta(N, \nu_{n_0})$$

with $\beta(N, \nu_{n_0})$ given in (5.27). It then follows for sufficiently large N that

$$|\operatorname{tr} \mathcal{K}^k - \operatorname{tr} \mathcal{K}_N^k| \leqslant ck\beta(N, \nu_{n_0}) \|\mathcal{K}\|_{\mathfrak{I}_p}^p.$$

Hence equation (5.26) follows. □

Observe from equation (5.26) and equation (5.24), that for a given eigenvalue z_0^{-1} of index $\nu \leqslant \nu_{n_0}$, we have for some sufficiently large N and $z \in \rho(\mathcal{K})$, that

$$|d_p(z_0) - d_{Np}(z_0)| \leqslant |d_p(z) - d_{Np}(z)|. \tag{5.28}$$

Corollary 5.1. *Let the integral operator $\mathcal{K}$ be in $\mathfrak{I}_p$ and let the set of operators $\{\mathcal{K}_N\}_{N \geqslant 1}$ be collectively compact. Assume that $\mathcal{K}$ has simple eigenvalues λ_n, and that the basis eigenfunctions $\{u_n\}$ are either purely real or imaginary. Then for some sufficiently large N and for all $z \in \mathbb{C}$ and $c > 0$, we have*

$$|d_p(z) - d_{Np}(z)| \leqslant c\|\mathcal{K}u_1 - \mathcal{K}_N u_1\|, \tag{5.29}$$

where $\|\mathcal{K}u_1 - \mathcal{K}_N u_1\| = \sup_{n \geqslant 1} \{\|\mathcal{K}u_n - \mathcal{K}_N u_n\|\}$

Indeed since for all $n \geqslant 1$, eigenvalues λ_n of $\mathcal{K}$ are simple, it follows that their corresponding indices ν_n are equal to 1 (index of an eigenvalue is less than or equal to its algebraic multiplicity). Since for all $n \geqslant 1$, the regularity of eigenfunctions u_n associated with the compact integral operator $\mathcal{K}$ is the same, it follows, for example

$n = 1$, that

$$\|\mathcal{K}u_1 - \mathcal{K}_N u_1\| = \sup_{n\geqslant 1}\{\|\mathcal{K}u_n - \mathcal{K}_N u_n\|\}.$$

For $n > 1$, we have that $\|\mathcal{K}u_n - \mathcal{K}_N u_n\| = O\big(\|\mathcal{K}u_1 - \mathcal{K}_N u_1\|\big)$. It follows from (5.24), (5.26) and (5.28) that

$$|d_p(z) - d_{Np}(z)| = c|d_p(z_n) - d_{Np}(z_n)|,$$

where $z_n^{-1} \in \sigma(\mathcal{K})$. Hence equation (5.29) follows. In other words, Corollary 5.1 tells us that for $z^{-1} \in \sigma(\mathcal{K})$ or $z \in \rho(\mathcal{K})$, the rate of convergence in computing the p-modified Fredholm determinants associated with $\mathcal{K}$ is the same, up to a nonzero constant (cf. Figure 5.1).

Remark 5.6. If λ_n are semisimple then their indices ν_n are equal to 1 (mentioned as an exercise in Meyer [54, p. 596]). However the rate of convergence will not be the same for all $z \in \mathbb{C}$ like in Corollary 5.1. Instead, the maximum error in (5.26) as well as (5.24), will depend on the propreties of each corresponding eigenfunction (e.g. parity, regularity, etc). We encounter this situation in the case of self-adjoint and normal operators with semisimple eigenvalues, for example (see Example 5.3 and 5.2).

Remark 5.7. Suppose for example that $\mathcal{K}$ in Corollary 5.1 is associated with a kernel which has a jump discontinuity in the first derivative on the diagonal. Then for a given quadrature method which integrates through the discontinuity region, the rate of convergence is the same for all $z \in \mathbb{C}$ like in Corollary 5.1. However, if the method takes into account the discontinuity, we might expect better convergence for $z_0^{-1} \in \sigma(\mathcal{K})$ than for $z \in \rho(\mathcal{K})$ (cf. Figure 5.1).

5.3 Numerical Results

In this section we numerically evaluate the p-modified Fredholm determinants associated with the integral operator $\mathcal{K}$ given by (5.2), where its corresponding kernel is

given, for all $x, y \in [a, b] \subset \mathbb{R}$, by

$$k(x,y) = \begin{cases} k^{(1)}(x,y), & a \leqslant y \leqslant x \\ k^{(2)}(x,y), & x < y \leqslant b. \end{cases} \tag{5.30}$$

The functions $k^{(1)}$ and $k^{(2)}$ are the restrictions of the kernel k in the lower and upper triangular domains of the square $[a, b] \times [a, b]$. We follow Kang et al.'s [43] method (see below) for solving Fredholm integral equations of second kind, since it leads to high accuracy when computing the zeros of Fredholm determinants, in particular for integral operators with semi-separable kernel. For weakly singular kernels (cf. Example 5.4), the interpolation method described in Section 5.2 will be used to compute eigenvalues associated with the integral operator $\mathcal{K}$. We briefly give the construction of the method of Kang et al. Assume that $k^{(1)}(x, y)u(y)$ and $k^{(2)}(x, y)u(y)$ can be approximated by Chebyshev polynomials $T_n(x)$, i.e. for fixed $x_m \in [-1, 1]$ (a map from $[a, b] \to [-1, 1]$) and $m = 1, \cdots, N$,

$$k^{(1)}(x_m, y)u(y) = \sum_{n=0}^{N} a_{mn} T_n(y)$$

$$k^{(2)}(x_m, y)u(y) = \sum_{n=0}^{N} \tilde{a}_{mn} T_n(y),$$

where the a_{mn} and $\tilde{a}_{mn}$ are real-valued constants. Then we replace the eigenvalue problem (5.1) by (cf. [43])

$$\left(\mathrm{id}_N + z\frac{1}{2}\left(CS_rC^{-1} \circ A_1 + CS_lC^{-1} \circ A_2 \right) \right) \mathbf{u} = 0, \tag{5.32}$$

where $\circ$ denotes pointwise multiplication, S_r, S_l are the right and the left spectral integration matrix respectively (see Appendix B), $C = \left(T_n(x_m)\right)_{n,m=0}^{N}$, $A_1 = \left(k^{(1)}(x_m, x_n)\right)_{n,m=0}^{N}$, $A_2 = \left(k^{(2)}(x_m, x_n)\right)_{n,m=0}^{N}$ and $\mathbf{u} = \left(u(x_1), \ldots, u(x_N)\right)^T$.

One of the advantages of using Chebyshev polynomials is that the coefficients in the expansion of an indefinite integral can be easily obtained from that of the series expansion of the integrand in terms of the Chebyshev polynomial [16]. With this property, the Chebyshev polynomials are extremely useful for integral equations associated with

kernel functions having jump discontinuity along the diagonal. In all our examples below, we use the Nyström–Clenshaw–Curtis and the Nyström–Gauss–Legendre referred to NCC as in [43] and NGL, respectively. The latter method integrates through the discontinuity of the kernel k, since it approximates the function $k(x,y)u(y)$, for all $y \in [-1,1]$ and fixed $x \in [-1,1]$. Hence, this results in a poor convergence compared to the NCC which does not integrate through the discontinuity because it approximates each function $k^{(i)}(x,y)u(y)$ for all $y \in [-1,1]$, fixed $x \in [-1,1]$ and $i = 1,2$.

Example 5.1. For our first example, we consider the problem studied by Bornemann in [10], i.e.

$$u = z\mathcal{K}u, \tag{5.33}$$

where, for all $x, y \in [0,1]$, the kernel k of the integral operator $\mathcal{K}$ is given by

$$k(x,y) = \begin{cases} x(1-y), & x \leqslant y \\ y(1-x), & y < x. \end{cases}$$

Our goal here is not to compute the Fredholm determinant, but to emphasise Corollary 5.1 and Remark 5.7. For this example, the operator $\mathcal{K}$ is trace class and self-adjoint. The corresponding set of operators $\{\mathcal{K}_N\}_{N\geq 1}$ is collectively compact since k is continuous (cf. [3]). The eigenvalues of $\mathcal{K}$ are simple and are given, for all $n = 1, 2, \ldots,$ by

$$z_n^{-1} = \lambda_n = \frac{1}{\pi^2 n^2}.$$

Accordingly, Corollary 5.1 tells us that the rate of convergence in evaluating the Fredholm determinant at the spectrum and the resolvent set are the same up to a nonzero positive constant. The rate of convergence for this example is $O(N^{-2})$ (cf. [10]), for the NGL. Indeed this is seen in Figure 5.1 where we display the error $|d(z) - d_N(z)|$ computed by the NGL and the NCC methods at the eigenvalue, $z_1 = \lambda_1^{-1} = \pi^2$ and at $z = 1$. At the eigenvalue, the NCC method converges very fast as N gets bigger (see Figure 5.1 (left)). In fact, the accuracy for the NCC method reaches machine precision for just $N = 16$, but at $z = 1$ it converges at the rate of $O(N^{-2})$ (see Figure 5.1 (right)). We recall that at the roots z_n, the p-Fredholm determinants $d_p(z_n) = 0$ so that the error is just $|d_{Np}(z_n)|$.

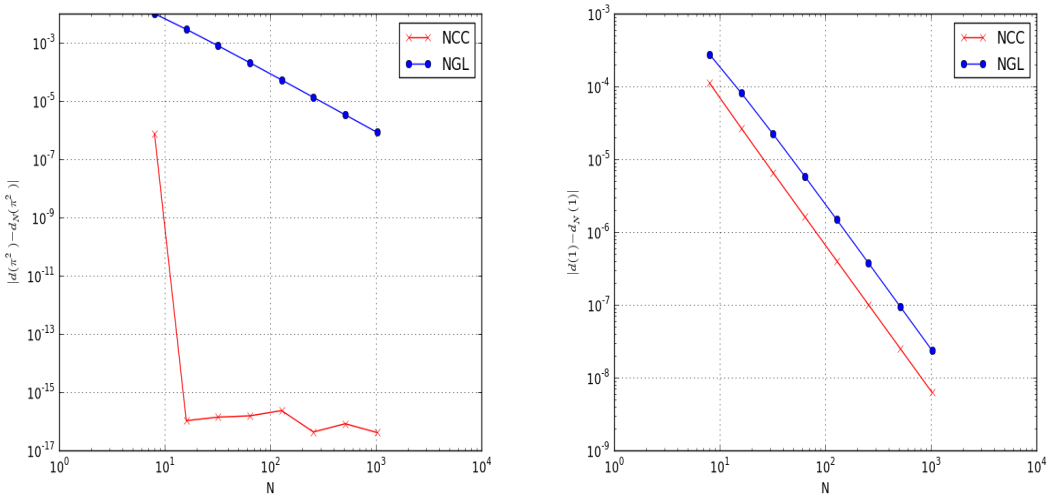

Figure 5.1: $\log_{10}$ of the error evaluated at $z_1 = \lambda_1^{-1} = \pi^2$ (left) and at $z = 1$ (right) of Example 5.1.

Example 5.2. Our goal in this example is to show that for a self-adjoint operator with semi-simple eigenvalues, Corollary 5.1 does not hold, i.e. the rate of convergence in evaluating the Fredholm determinant at the spectrum and at the resolvent set are not the same for the NGL method. The kernel function associated with the integral operator $\mathcal{K}$ is given, for all $x, y \in [0, 1]$, by

$$k(x, y) = \frac{1}{12} - \frac{1}{2}|x - y| + \frac{1}{2}(x - y)^2.$$

The operator $\mathcal{K}$ is self-adjoint with eigenvalues given by (cf. [38])

$$z_n^{-1} = \lambda_n = \frac{1}{4n^2\pi^2}, \ n = 1, 2, \ldots .$$

Since $\sum_{n=1}^{\infty} |\lambda_n| = \|\mathcal{K}\|_{\mathfrak{I}_1} < \infty$, the operator $\mathcal{K}$ is of trace class and its corresponding Fredholm determinant is

$$d(z) = \prod_{n=1}^{\infty} \left(1 - \frac{z}{4n^2\pi^2}\right) = \left(\frac{\sin(\sqrt{z}/2)}{\sqrt{z}/2}\right)^2.$$

For $n \geqslant 1$, each eigenvalue λ_n has an algebraic multiplicity $m_n = 2$ with index $\nu_n = 1$ (cf. Theorem 5.3) since $\mathcal{K}$ is self-adjoint operator. Therefore following the same line of arguments (in particular, the hat like shape of a section of the kernel k) of Bornemann

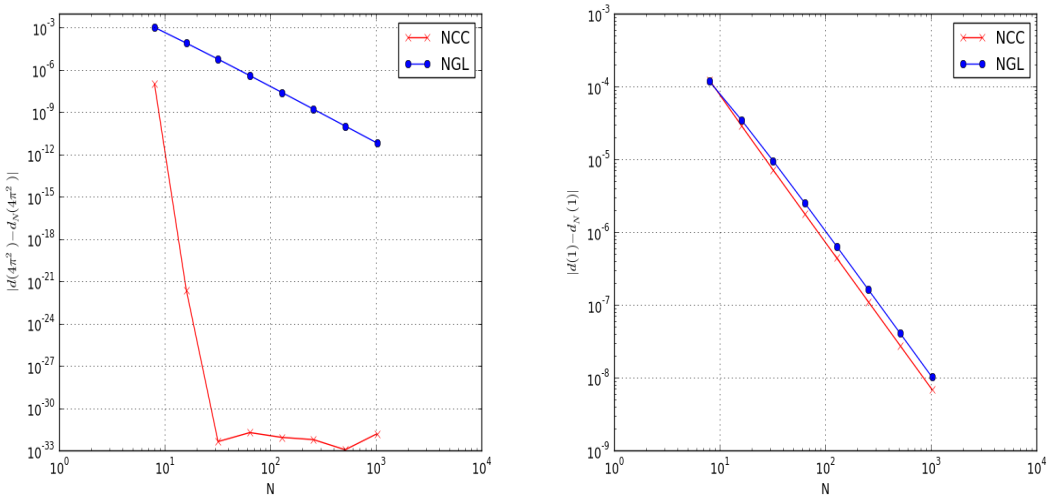

Figure 5.2: $\log_{10}$ of the error evaluated at $z_1 = \lambda_1^{-1} = 4\pi^2$ (left) and at $z = 1$ (right) for Example 5.2.

in [10] which led to an error of order $O(N^{-2})$ in Example 5.1, we conclude that

$$\begin{aligned}\beta(N,1) &= \max\{\|\mathcal{K}u_{1n} - \mathcal{K}_N u_{1n}\|, \|\mathcal{K}u_{2n} - \mathcal{K}_N u_{2n}\|\} \\ &= O(N^{-2}),\end{aligned}$$

where, for $n \geqslant 1$, the eigenfunctions $u_{1n}(x) = \sqrt{2}\cos(2n\pi x)$ and $u_{2n}(x) = \sqrt{2}\sin(2n\pi x)$ (cf. [38, Example 5, p. 74]) are associated with the eigenvalue λ_n. However we see from Figure 5.2 that the convergence error of the NGL method is $O(N^{-4})$ at the eigenvalue $z_1 = 4\pi^2$ (see Figure 5.2 (left)) whereas at $z = 1$ it is $O(N^{-2})$ (see Figure 5.2 (right)). The NCC method has the same error convergence as the previous example (see Figure 5.2). Note from Figure 5.2 that the rate of convergence for the NGL at the eigenvalue behaves like the square of the rate of convergence at the resolvent set. We also note that after the machine precision, the values in the vertical axis in Figure 5.2 (right) are squared, for the NCC. In conclusion, the error convergence at the spectrum and at the resolvent set are in general not the same for self-adjoint operators with semi-simple eigenvalues when using NGL method.

Example 5.3. Here we numerically compute a 2-modified Fredholm determinant. We also show that for a normal operator with simple eigenvalues and complex eigenfunctions, Corollary 5.1 does not hold. The kernel k associated with the integral operator

$\mathcal{K}$ is given, for all $x, y \in [-1, 1]$, by

$$k(x,y) = \begin{cases} 1, & y \leqslant x \\ -1, & x < y. \end{cases}$$

Note that k is of the form given in (5.7), where $g(x,y) = \text{sign}(x-y)$ and $h(x,y) = 1$. The integral operator $\mathcal{K}$ associated with the above kernel function is a Hilbert–Schmidt operator since $\|k\|_{L^2([-1,1]^2)} < \infty$ (see more details below), and it is a normal operator [3] as well, i.e. $\mathcal{K}^*\mathcal{K} = \mathcal{K}\mathcal{K}^*$. The coefficients $\alpha_n^{(2)}$ (cf. (2.20) of Chapter 2) in the expression of the 2-modified Fredholm determinant $d_2(z)$ are easily computed via (2.22) of Chapter 2 by setting $\operatorname{tr}\mathcal{K}$ to zero (Hilbert. [37]). They are given explicitly, for $q = 0, 1, 2, \ldots$, by

$$\alpha_n^{(2)} = \frac{1}{n!} \begin{cases} 2^n, & n = 2q \\ 0, & n = 2q+1. \end{cases}$$

Hence the 2-modified Fredholm determinant is

$$d_2(z) = \cosh(2z) \tag{5.34}$$

with simple pure imaginary zeros z_k satisfying

$$z_n^{-1} = \lambda_n = -i\frac{4}{\pi}\frac{1}{2n+1}, \quad n \in \mathbb{Z}. \tag{5.35}$$

The eigenfunctions u_n associated with the eigenvalues λ_n are given by

$$u_n(x) = \frac{1}{\sqrt{2}} \exp\left(i\pi(2n+1)x/2\right). \tag{5.36}$$

From (5.35), it is clear that the trace of $\mathcal{K}$ is divergent but the trace of $\mathcal{K}^2$ is convergent, i.e.

$$\operatorname{tr}\mathcal{K}^2 = -2\frac{16}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2} = -4. \tag{5.37}$$

The factor of 2 before the sum in (5.37) comes from the fact that $\bar{\lambda}_n$ (conjugates of λ_n) are also eigenvalues of $\mathcal{K}$, i.e. $d_2(\bar{z}_n) = d_2(z_n) = 0$ for all $n \in \mathbb{Z}$. Hence

[3] The kernel k_2 of $\mathcal{K}\mathcal{K}^*$ given by (5.38) satisfies $k_2 = k_2^*$.

$\sum_{n\geqslant 0} \lambda_n^2 + (\bar{\lambda}_n)^2 = 2\sum_{n\geqslant 0} \lambda_n^2$. Equivalently, the determinant in (5.34) is given by

$$d_2(z) = \prod_{n=0}^{\infty} \left[\Big(1 - i4z/\pi(2n+1)\Big) \exp\Big(i4z/\pi(2n+1)\Big) \right].$$

For plotting the approximation of $d_2(z)$, we compute the determinant of the linear

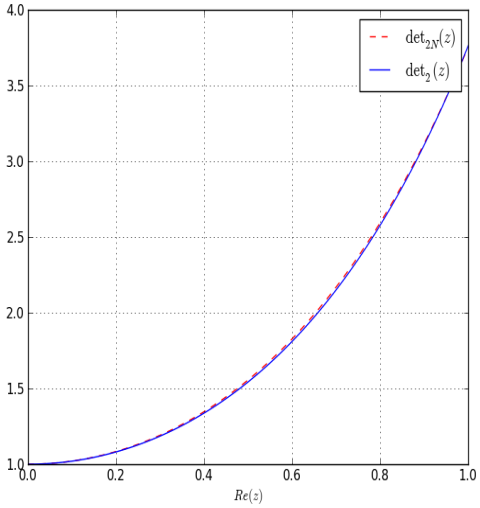

Figure 5.3: The graph of $d_2(z)$ and $d_{2N}(z)$, for real values of z and $N = 30$.

system arising from applying the Nyström-rectangular rule to the integral equation (5.33). In Figure 5.3, we display the finite dimensional determinant $d_{2N}(z)$ and the 2-modified Fredholm determinant $d_2(z)$, for real values of $z \in [0, 1]$.

Note that the eigenfunctions (5.36) of $\mathcal{K}$ have nonzero real/imaginary parts. Hence Corollary 5.1 does not hold for the operator $\mathcal{K}$. In fact, it is seen in Figure 5.4 (left) and (right) that the rate of convergence of $\big|d_2(z) - d_{2N}(z)\big|$ at $z_0 = \lambda_0^{-1} = i\pi/4 \in \sigma_d(\mathcal{K})$ and at $z = 1 \in \rho(\mathcal{K})$ is $O(N^{-2})$ and $O(N^{-1})$ respectively. The rate of $O(N^{-1})$ was expected due to the discontinuity of the kernel k.

To implement the strategy mentioned in the paragraph preceding Theorem 5.1, we compute the iterated integral operator. The 2-iterated kernel, k_2 of this example, is

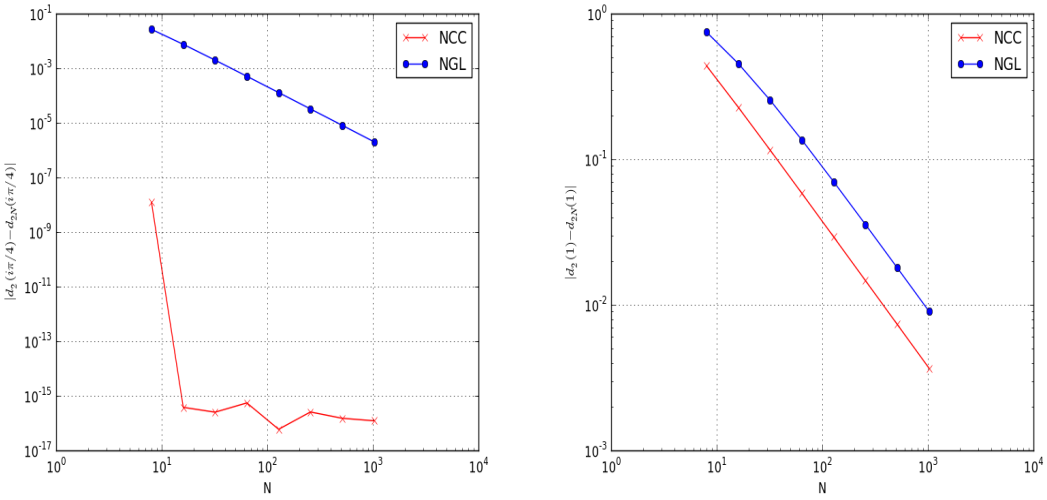

Figure 5.4: $\log_{10}$ of the error evaluating at $z_1 = \lambda_1^{-1} = i\pi/4$ (left) and at $z = 1$ (right) for Example 5.3.

continuous Hermitian, and it is given, for all $x, y \in [-1, 1]$, by

$$k_2(x, y) = -2 + 2|x - y|. \tag{5.38}$$

The integral operator $\mathcal{K}^2$ associated with the kernel k_2 is of trace class since k_2 satisfies Item 3 defining trace class operators of Subsection 2.3.1 in Chapter 2 with $\alpha > 1/2$. Therefore its trace $\operatorname{tr} \mathcal{K}^2$ in (5.37) is also given by (cf. [68] and [38])

$$\begin{aligned} \operatorname{tr} \mathcal{K}^2 &= \int_{-1}^{1} k_2(x, x) \mathrm{d}x \\ &= \int_{-1}^{1} \int_{-1}^{1} k(x, y) k(y, x) \mathrm{d}x \mathrm{d}y = -4. \end{aligned}$$

The coefficients in the Fredholm determinant series of $\mathcal{K}^2$ are given, for all $q \geqslant 1$, by $\alpha_{2q}^{(1)} = 4^{2q}/2(2q)!$ and $\alpha_0^{(1)} = 1$. Hence, the Fredholm determinant associated with the operator $\mathcal{K}^2$ is

$$\det_1\big(\mathrm{id} - z^2 \mathcal{K}^2\big) = \frac{1}{2}(\cosh(4z) + 1). \tag{5.39}$$

Since $d_2(z) = d_2(-z)$, we must have from Theorem 5.1 that

$$(d_2(z))^2 = \det_1\big(\mathrm{id} - z^2 \mathcal{K}^2\big). \tag{5.40}$$

Indeed the above equality holds because

$$(\cosh(2z))^2 = \frac{1}{2}(\cosh(4z) + 1).$$

Note that due to the discontinuity in the kernel function k, the approximation $d_{2N}(z)$ converges slowly to $d_2(z)$. Since relation (5.40) holds and that k_2 is continuous, one can improve the order of convergence in computing $d_2(z)$ by approximating $\det_1(\mathrm{id} - z^2\mathcal{K}^2)$ instead.

Remark 5.8. The same behaviour of the error holds for the self-adjoint operator $i\mathcal{K}$ with eigenvalues $\pm i\lambda_n$, as well.

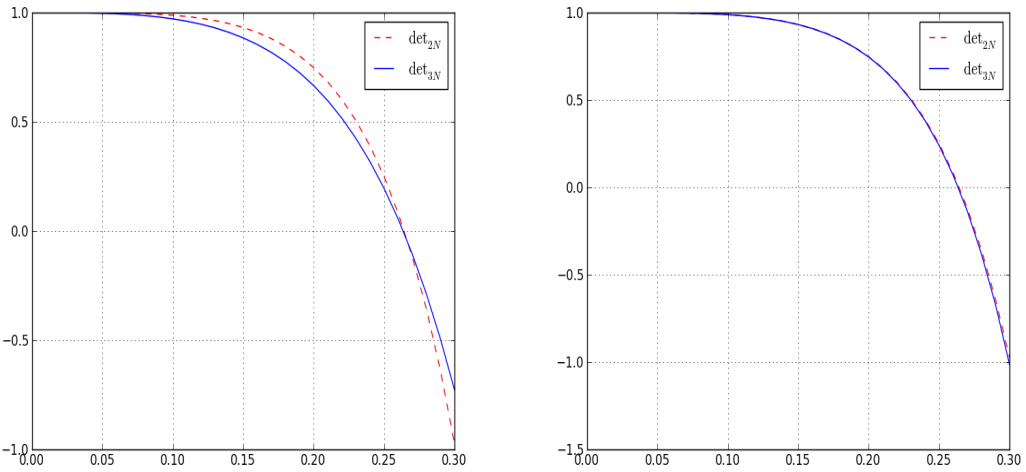

Figure 5.5: The graphs of $d_{3N}(z)$ and $d_{2N}(z)$ (left) and $d_{2N}(z)d_{2N}(-z)$ and $d_{3N}(z)$ (right), for real values of $z \in [0, 0.3]$ and $N = 30$.

Example 5.4. In this example, we compute the 3-modified Fredholm determinant. Numerically, we shall observe the uniform convergence of Theorem 5.2. For all $x, y \in [-1, 1]$ and $\alpha \in [0, 1[$, the kernel $k(x, y)$ associated with the integral operator $\mathcal{K}$ is given by

$$k(x, y) = \frac{1}{|x - y|^\alpha}.$$

The kernel function $k(x, y)$ is of the form given in (5.7) with $h(x, y) = 1$. Hence the integral operator $\mathcal{K}$ associated with the above kernel is compact and positive definite,

self-adjoint operator [5]. In particular, for $0 < \alpha < 1/2$ the integral operator $\mathcal{K}$ is Hilbert–Schmidt (cf. [38] and [8]). Therefore, the 2-modified Fredholm determinant is computed as in Example 5.3 by substituting zero in the kernel function at $x = y$ [37]. For this reason, we shall only focus on the case $\alpha = 1/2$. For this particular case, the integral operator $\mathcal{K}$ is not Hilbert–Schmidt operator since $\|k\|_{L^2([-1,1]^2)}$ is unbounded, it is possibly in $\mathfrak{I}_p$ for $p \geqslant 3$. The 3-iterated kernel k_3 is continuous (cf. [8]), and the corresponding integral operator $\mathcal{K}^3$ is a positive definite, self-adjoint operator. In fact the positiveness and the self-adjointness of $\mathcal{K}^3$ follow from that of $\mathcal{K}$. From Item 4 defining trace class operators of Subsection 2.3.1 in Chapter 2, it follows that $\mathcal{K}^3$ is of trace class with

$$\operatorname{tr} \mathcal{K}^3 = \int_{-1}^{1} k_3(x,x)\mathrm{d}x = \|\mathcal{K}^3\|_{\mathfrak{I}_3} < \infty.$$

Since $\mathcal{K}$ is positive definite, self-adjoint operator, it implies that

$$\|\mathcal{K}\|_{\mathfrak{I}_3}^3 = \operatorname{tr} |\mathcal{K}|^3 = \operatorname{tr} \mathcal{K}^3 < \infty.$$

Hence the integral operator $\mathcal{K}$ is in $\mathfrak{I}_3$. For the numerical computation of the 3-modified Fredholm determinant $d_3(z) = \det_3(\mathrm{id} - z\mathcal{K})$, we need to compute numerically the eigenvalues of $\mathcal{K}$ and form the finite dimensional version of equation (2.23) of Chapter 2. However given Theorem 5.1 we are not required to, we only need to have an explicit expression of the 2-iterated kernel k_2 and set its diagonal values to zero. Using Maple, the 2-iterated kernel k_2 is given, for all $x, y \in [-1, 1]$, by

$$k_2(x,y) = \begin{cases} -\ln\left(2 - y - x - 2\sqrt{(1-y)(1-x)}\right) + \pi \\ \quad + \ln\left(2 + y + x + 2\sqrt{(1+y)(1+x)}\right), & x < y \\ -\ln\left(2 + y + x - 2\sqrt{(1+y)(1+x)}\right) + \pi \\ \quad + \ln\left(2 - y - x + 2\sqrt{(1-y)(1-x)}\right), & x > y. \end{cases}$$

In Figure 5.5 (left), we display the approximation $d_{3N}(z)$ of $d_3(z)$ computed using the five eigenvalues of largest modulus and the approximation $d_{2N}(z)$ of $\det_2\big(\mathrm{id} - z\mathcal{K}^2\big)$ obtained by applying the Nyström-rectangular rule on the eigenvalue problem. In Figure 5.5 (right), we display $d_{2N}(z)d_{2N}(-z)$ and $d_{3N}(z)$. Clearly we see that the product $d_{2N}(z)d_{2N}(-z)$ coincides with $d_{3N}(z)$ which confirm Theorem 5.1. Therefore,

eigenvalues of $\mathcal{K}$ can be deduced from those of $\mathcal{K}^2$.

5.4 Concluding remarks

In this chapter, we have given theoretical and numerical results concerning the approximation error $(d_p - d_{Np})$, where d_p is the p-modified Fredholm determinants and d_{Np} is the finite dimensional determinants associated with d_p. These results are as follows: first, we have shown that the approximation error $(d_p - d_{Np})$ is uniform in a bounded domain. Second, we have given the rate of convergence when evaluating $(d_p - d_{Np})$ lies in the spectrum or in the resolvent set. As a consequence, we have observed that numerical evaluation of the p-modified Fredholm determinants is nothing other than an interpolation in which the interpolation points are the eigenvalues of the operator $\mathcal{K}$. Although we dealt with a bounded domain of $\mathbb{R}$, an extension of the present analysis to a bounded subset of $\mathbb{R}^n$ is possible. This is of course under the assumption that the $\mathcal{K}$ is compact and that the set $\{\mathcal{K}_N\}_{N\geqslant 1}$ is collectively compact.

Chapter 6

Computing Fredholm determinants for travelling wave problems

6.1 Introduction

This chapter aims at numerically compute the Fredholm determinant associated with travelling wave problems, and then compare its accuracy with that of the Evans function. The numerical evaluation of the Fredholm determinant here differs slightly from that of the previous chapter, since the underlying integral operator $\mathcal{K}(\lambda)$ is not linear in λ. Consequently, one needs to compute the matrix approximating the integral equation for each value of $\lambda \in \Lambda \subset \mathbb{C}$. This might seem a disadvantage but since exponential convergence can be achieved for smooth kernels when applying the Nyström-quadrature methods, and moreover since the Fredholm determinants extend naturally to higher dimensions, it is then an interesting direction to pursue.

Numerically the Evans function can be difficult to compute due to different exponential growth of solutions in the semi-bounded intervals. However, this can be resolved once the problem is expressed in an exterior algebra framework (see [14]). Unfortunately the size of the new problem increases exponentially with the order of the original problem. Methods such as continuous-orthogonalisation [40] or Grassmannian-shooting (cf. [52]) resolve this problem of high dimensionality. When computing the Fredholm determinant, these issues do not arise.

To compute the eigenfunctions for general problems, one usually needs to compute the eigenvalues first. This can be achieved by the shooting method—fix a boundary condition and integrate the problem for different values of λ until the other boundary condition is matched. By doing so, both eigenvalues and eigenfunctions are simultaneously computed. A further alternative involves approximating the differential equations by a system of algebraic equations and then computing the eigenvalues and eigenvectors of the corresponding matrix. However, since the essential spectrum of the differential operator is not empty (in our case), one needs to refine the (uniform) meshgrids in order to track the isolated non-moving points (eigenvalues) in the complex plane, for the finite differences method. In the integral formulation, the computation of the eigenfunctions is almost identical to the shooting method. That is, in order to convert the differential problem into an integral equation, an appropriate construction of the Green's function is needed. In the travelling wave problems, this corresponds to the projection of the evolution onto the stable/unstable subspaces. Therefore any nontrivial square integrable solution is an eigenfunction associated with a nonzero eigenvalue. This follows from the compactness property of the underlying integral operator. The analogy with the shooting method is that the eigenfunctions satisfy suitable boundary conditions which follow from the Green's function.

To compute the Fredholm determinants numerically, the integral equation is approximated by a system of algebraic equations whose determinant is then computed. In this chapter, the Nyström-type quadrature methods considered to reduce the integral equation to a system of equations are the following:

1. Gaussian quadrature in an unbounded domain;
2. Truncation of the domain and application of the trapezoidal rule; and
3. Mapping of the infinite domain to a finite one and application of Gaussian quadrature.

For a kernel function with a jump discontinuity in the first derivative, Nyström-product-integration based on Lagrange interpolation is considered. This allows us to generate a method whose rate of convergence is comparable to that of the Runge–Kutta method of order four, depending on the smoothness of the function of course.

However for a sufficiently smooth kernel, the Nyström-trapezoidal rule is applied since it is computationally less expensive than product-integration or Gaussian quadratures, for an equivalent convergence rate. methods which are, in our case, the step size.

6.2 The numerical approach

In this section, the numerical approach that we use for computing the Fredholm determinant associated with the travelling waves is presented. We approximate the integral equation by a system of linear algebraic equations arising from applying a Nyström-type method [55]. We then compute its determinant.

Since our concern is to compute eigenvalues associated with the travelling wave problems, we recall that the underlying kernel k satisfies, for a given perturbation $v \in L^1$, $\lambda \in \Lambda \subset \mathbb{C}$, some constants $c > 0$ and $\kappa > 0$ and for all $x, y \in \mathbb{R}$ (cf. (4.19) of Chapter 4), the following inequality

$$\big|k(x, y; \lambda)\big| \leqslant c\, v(x) \mathrm{e}^{-\kappa|x-y|} \tilde{v}(y), \tag{6.1}$$

where $\tilde{v} = v|v|^{-1/2}$. With the above condition, the underlying integral operator $\mathcal{K}(\lambda)$ is compact in $L^2(\mathbb{R})$, i.e. $\mathcal{K}(\lambda) \in \mathfrak{I}_2$, since $k \in L^2(\mathbb{R}^2 \times \Lambda, \mathbb{C})$ (cf. (4.21) of Chapter 4). Furthermore, for all $u \in L^2(\mathbb{R})$, $x_1, x_2 \in \mathbb{R}$ and $\lambda \in \Lambda$, we have

$$|\mathcal{K}(\lambda)u(x_1) - \mathcal{K}(\lambda)u(x_2)| \leqslant \|u\|_{L^2} \Big(\int_{\mathbb{R}} |k(x_1, y; \lambda) - k(x_2, y; \lambda)|^2 \mathrm{d}y \Big)^{1/2}.$$

Hence for the integral eigenvalue problem $K(\lambda)$ maps $L^2(\mathbb{R})$ into the space of functions in $L^2(\mathbb{R})$ which are continuous, i.e. $C(\mathbb{R}) \cap L^2(\mathbb{R})$.

Remark 6.1. The analysis that we carry out holds for kernel $k \colon \mathbb{R}^2 \times \Lambda \to \mathbb{C}^{n \times n}$, where the absolute value $|\cdot|$ is replaced by the norm of a matrix $\|\cdot\|_{\mathbb{C}^{n\times n}}$ or the norm of a vector $\|\cdot\|_{\mathbb{C}^n}$ for $ku \colon \mathbb{R}^2 \times \Lambda \to \mathbb{C}^n$ accordingly.

As in the previous chapter, we assume that the kernel function k is given by

$$k = g \times h \tag{6.2}$$

where the function g is analytic in λ such that the above product is in $L^2(\mathbb{R}^2 \times \Lambda, \mathbb{C})$, and h is continuous and analytic in $\mathbb{R}^2 \times \Lambda$ satisfying

$$\sup_{(x,y)\in\mathbb{R}^2} \big|h(x, y; \lambda)\big| < \infty. \tag{6.3}$$

Note that the advantage of assuming k of the form (6.2) is to include more general function spaces and hence extend the quadrature methods for continuous functions to such spaces.

If we assume that the above function k in (6.2) is continuous in $\mathbb{R} \times \mathbb{R}$, then Gauss–Hermite quadrature might not be the best choice since the exponential decay of the kernel k is slower than that of Hermite functions. Therefore, to solve the integral equation

$$\big(\mathrm{id} - \mathcal{K}(\lambda)\big)u = 0,$$

for all $u \in L^2$ and $\lambda \in \Lambda$, we proceed either by truncating the domain or transforming the unbounded domain to a finite one and then apply the appropriate Gauss-quadrature.

6.2.1 Domain truncation

For kernel functions satisfying the exponential decay in (6.1), truncation methods might be more effective than applying a Gaussian quadrature either for unbounded domain or (finite) truncated domain. To this end, for some suitable chosen $R > 0$ (truncation point), $\lambda \in \Lambda,\ x \in [-R, R]$, we define the operator $\mathcal{K}_{R,N}(\lambda)$ by

$$\mathcal{K}_{R,N}(\lambda)u(x) = \sum_{j=1}^{N} w_j(x, \lambda)h(x, y_j; \lambda)u(y_j), \tag{6.4}$$

where $\{y_j\}$ are the nodal points in $[-R, R]$ and

$$w_j(x, \lambda) = \int_{-R}^{R} g(x, y; \lambda)P_j(y)\mathrm{d}y \tag{6.5}$$

with P_j is a polynomial interpolation of order j. We also define the truncated integral operator $\mathcal{K}_R(\lambda)$, for all $x \in [-R, R]$ and $\lambda \in \Lambda$, by

$$\mathcal{K}_R(\lambda)u(x) = \int_{-R}^{R} k(x, y; \lambda)u(y)\mathrm{d}y, \tag{6.6}$$

and assume, for sufficiently large N and for $x \in [-R, R]$, that

$$\mathcal{K}_R(\lambda)u(x) \approx \mathcal{K}_{R,N}(\lambda)u(x). \tag{6.7}$$

Since $k \in L^2(\mathbb{R}^2 \times \Lambda, \mathbb{C})$ (i.e. $\mathcal{K}(\lambda) \in \mathfrak{I}_2$), we choose the functions g so that the function $w_j(\cdot, \lambda)$ is continuous, for $j = 1, \dots N$ and $\lambda \in \Lambda$. Consequently the set of operators $\{\mathcal{K}_{R,N}(\lambda)\}_{N \geqslant 1}$ is collectively compact in the set of bounded linear operators in $C[-R, R]$. We omit the proof since it is the same as in the previous chapter.

Suppose for instance that $\mathcal{K}(\lambda) \in \mathfrak{I}_1$, and we denote by $d(\lambda)$ its corresponding Fredholm determinant. We also denote by $d_R(\lambda)$ the Fredholm determinant of the restricted operator $\mathcal{K}_R(\lambda)$ in $C[-R, R]$ and $d_{R,N}(\lambda)$ its approximation. Let λ_0 be an eigenvalue of the operator $\big(\mathrm{id} - \mathcal{K}(\lambda)\big)$. We now show, for some $R > 0$, that the error $\big|d(\lambda_0) - d_{N,R}(\lambda_0)\big|$ is very small as N goes to infinity. Since $\{\mathcal{K}_{R,N}(\lambda)\}_{N \geqslant 1}$ is collectively compact, we have, for fixed $\lambda \in \Lambda$ and sufficiently large N, that (Anselone. [3, Proposition 1.7])

$$\|\mathcal{K}_R(\lambda)u - \mathcal{K}_{R,N}(\lambda)u\| \leqslant \epsilon/2. \tag{6.8}$$

On the other hand, given that $k \in L^2(\mathbb{R}^2 \times \Lambda, \mathbb{C})$, we have, for $u \in C(\mathbb{R}) \cap L^2(\mathbb{R})$ and $\lambda \in \Lambda$,

$$\begin{aligned}
\|\mathcal{K}(\lambda)u - \mathcal{K}_R(\lambda)u\|_{L^2}^2 &\leqslant \int_{|x|>R} \left(\int_{|y|>R} |k(x, y, \lambda)u(y)|\mathrm{d}y \right)^2 \mathrm{d}x \\
&\leqslant \|u\|_{L^2(\mathbb{R}\setminus[-R,R])}^2 \int_{|x|>R} \int_{|y|>R} |k(x, y, \lambda)|^2 \mathrm{d}y\mathrm{d}x \\
&\leqslant \epsilon^2/4.
\end{aligned} \tag{6.9}$$

Hence combining (6.8) and (6.9) we have, for $u \in C(\mathbb{R}) \cap L^2(\mathbb{R})$, some large N and $\lambda \in \Lambda$, that

$$\|\mathcal{K}(\lambda)u - \mathcal{K}_{R,N}(\lambda)u\| \leqslant \epsilon.$$

Suppose that $k \in C(\mathbb{R}^2 \times \Lambda) \cap L^2(\mathbb{R}^2 \times \Lambda)$ and (6.4) is reduced to the trapezoidal rule. Then if $y \mapsto k(x, y; \lambda)$ is twice differentiable, we have, for all $\lambda \in \Lambda$, a positive constant c and a suitably chosen $R > 0$, the well-known upper bound

$$\big\|\mathcal{K}(\lambda)u - \mathcal{K}_{R,N}(\lambda)u\big\| \leqslant \frac{c}{N^2}.$$

Given the estimate (6.8), we have, for some suitably chosen R and sufficiently large N, (recall that $d(\lambda_0) = 0$ and that $|d_R(\lambda_0)| \leqslant \epsilon$ which follows from (6.9)) that

$$\begin{aligned} |d(\lambda_0) - d_{N,R}(\lambda_0)| &\leqslant |d_R(\lambda_0)| + |d_R(\lambda_0) - d_{N,R}(\lambda_0)| \\ &\leqslant c \max_{i=1,\dots,m} \{\|\mathcal{K}_R(\lambda_0)u_i - \mathcal{K}_{R,N}(\lambda_0)u_i\|^{1/\nu}\}, \end{aligned}$$

where ν and m are the index and the algebraic multiplicity of the eigenvalue 1 of $\mathcal{K}(\lambda)$ respectively and $\{u_1, \cdots, u_m\}$ is a basis for $\mathrm{Ker}\big(\mathcal{K}(\lambda) - \mathrm{id}\big)^{\nu}$ (cf. [5, 6], or see Chapter 5).

Remark 6.2 (Domain mapping)**.** Assume that $k \in C(\mathbb{R}^2 \times \Lambda) \cap L^2(\mathbb{R}^2 \times \Lambda)$, and let (a, b) be an interval of $\mathbb{R}$. Given a smooth transformation $g\colon (a, b) \to \mathbb{R}$ such that

$$y = g(t),$$

the integral problem becomes

$$u(g(s)) = \int_a^b k(g(s), g(t); \lambda)u(g(t))\partial_t g(t)\mathrm{d}t.$$

Thus, the analysis of the previous chapter also applies here. We can then apply the Nyström-Gaussian quadratures method to the above integral equation. We use the Clenshaw–Curtis method for computing numerically integrals on the whole real line

$\mathbb{R}$, i.e. for some $L > 0$, we take $g(t) = L\cot(\mathrm{t}),\ t \in [0, \pi]$ and consider

$$\mathcal{K}_N(\lambda)u(x) = \sum_{j=1}^{N-1} w_j k(x, y_j; \lambda)u(y_j),$$

where $w_j = L\frac{\pi}{N}\partial_t g(t_j)$ and $t_j = j\pi/N$.

Clearly for simple eigenvalues and a suitably chosen R, the error in computing the Fredholm determinants for the truncation and mapping method (the above remark) differ by an $O(\epsilon)$. The product-integration method, i.e. (6.4) and (6.15), might be more advantageous since it allows using higher degree polynomial interpolation unlike Gaussian quadratures. Therefore if the kernel k is given by (6.2) with h sufficiently smooth, the product-integration may result in faster convergence than Gaussian quadratures (see next section).

6.3 Numerical results

Here we present some numerical results for the computation of the Fredholm determinants and the Evans function. We consider the scalar problem with perturbation v given by (4.37) (cf. Subsection 4.1.2 of Chapter 4). For the numerical evaluation of the Evans function, we use the Riccati–Runge–Kutta method (cf. [52]). For clarity, we present a brief explanation of the method. Assume that the matrices $Y^{\pm}$, solutions of the first order system that decay at $\pm\infty$ (cf. Chapter 3 or 4), are given by $Y^- = (u^- \quad v^-) \in \mathbb{C}^{n\times r}$ and $Y^+ = (u^+ \quad v^+) \in \mathbb{C}^{n\times(n-r)}$, where u^- and v^+ are invertible square matrices. Then the Evans function $E(\lambda)$ is given by

$$\begin{aligned} E(\lambda) &= \det_{\mathbb{C}^n}\left(\begin{pmatrix} \mathrm{id}_r & y^+(x,\lambda) \\ y^-(x,\lambda) & \mathrm{id}_{n-r}\end{pmatrix}\begin{pmatrix} u^- & O \\ O & v^+\end{pmatrix}\right) \\ &= \det_{\mathbb{C}^r} u^- \det_{\mathbb{C}^{n-r}} v^+ \det_{\mathbb{C}^{n\times n}}\begin{pmatrix} \mathrm{id}_r & y^+(x,\lambda) \\ y^-(x,\lambda) & \mathrm{id}_{n-r}\end{pmatrix} \end{aligned}$$

where O denotes the null matrix with appropriate size, $y^- = v^-(u^-)^{-1}$ and $y^+ = u^+(v^+)^{-1}$ satisfy Riccati equations as follows. Assume that

$$A(x,\lambda) = \begin{pmatrix} a(x,\lambda) & b(x,\lambda) \\ c(x,\lambda) & d(x,\lambda) \end{pmatrix},$$

where a, b, c and d are appropriate block matrices. Then the equations $\mathrm{d}Y^\pm/\mathrm{d}x = A(x,\lambda)Y^\pm$ become

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\begin{pmatrix} \mathrm{id} \\ y^- \end{pmatrix} u^-\right] = \begin{pmatrix} (a+by^-)u^- \\ (c+dy^-)u^- \end{pmatrix}.$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}x}y^- = c + dy^- - y^-(a+by^-) \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}x}u^- = (a+by^-)u^- \tag{6.10}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}x}y^+ = b + ay^+ - y^+(d+cy^+) \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}x}v^+ = (d+cy^+)v^+. \tag{6.11}$$

The Riccati equations are then given by the left-hand side of equations (6.10) and (6.11). They can be solved in the finite intervals $[\pm R, x^*]$, for example, by application of Runge–Kutta methods. We take $x^* = 0$ and carefully check that no singularities occur in the Riccati solutions. The product $\det_{\mathbb{C}^r} u^- \det_{\mathbb{C}^{n-r}} v^+$ is thus nonzero. Since we are interested in zeros of the Evans function, we compute

$$E(\lambda) \equiv \det_{\mathbb{C}^{n\times n}} \begin{pmatrix} \mathrm{id}_r & \hat{y}^+(0,\lambda) \\ \hat{y}^-(0,\lambda) & \mathrm{id}_{n-r} \end{pmatrix}. \tag{6.12}$$

In the following examples, we use the explicit Runge–Kutta method of order four (RK4). In our examples below, we consider travelling waves that are continuous and exponentially bounded, i.e. given a travelling wave ϕ, we have, for some constant $\beta > 0$,

$$\big|\phi(x)\big| \leqslant c\exp\left(-\beta|x|\right).$$

To compute the Fredholm determinant by the Nyström method based on the product-integration method, we take h and g in the expression of kernel k to be

$$h(x,y;\lambda) = f(\phi)(y),$$

where ϕ is the travelling wave, f a monomial function, and

$$g_0(x,y;\lambda) = \begin{cases} \sum_{j=1}^{r} \alpha_j \mathrm{e}^{\kappa_j^+(x-y)}, & x \leqslant y \\ \sum_{j=r+1}^{n} \alpha_j \mathrm{e}^{\kappa_j^-(x-y)}, & y < x, \end{cases} \tag{6.13}$$

with $\kappa_j^{\pm}$ the roots of the characteristic polynomial associated with the linear constant-coefficients differential operator $\big(\mathcal{L}_0 - \lambda \mathrm{id}\big)$ and $\alpha_j \in \mathbb{R}$ (cf. (4.40) and (4.41) of Chapter 4).

Typically, if one uses a linear interpolation, the right-hand side of (6.4) is

$$\sum_{j=0}^{N-1} \gamma_j(x,\lambda) f(\phi)(y_j) u(y_j) + \delta_j(x,\lambda) f(\phi)(y_{j+1}) u(y_{j+1}), \tag{6.14}$$

where $h_j = y_{j+1} - y_j$ and for $x_i \in \mathbb{R}$

$$\begin{aligned} \gamma_j(x_i,\lambda) &= \frac{1}{h_j} \int_{y_j}^{y_{j+1}} g_0(x_i,y;\lambda)(y_{j+1}-y)\mathrm{d}y \\ \delta_j(x_i,\lambda) &= \frac{1}{h_j} \int_{y_j}^{y_{j+1}} g_0(x_i,y;\lambda)(y-y_j)\mathrm{d}y. \end{aligned} \tag{6.15}$$

Let $C^{n+1}([a,b])$ denote the set of functions with $(n+1)$th continuous derivative in $[a,b] \subset \mathbb{R}$. As mentioned previously, we can apply the trapezoidal rule on the integral operator over a finite domain. Alternatively, we could map the infinite domain to a finite one and then use an appropriate Gaussian quadrature. For $n \geqslant 2$ in (6.13), both methods are satisfactory since the Green's function g_0 in (6.13) is $(n-2)$th continuously differentiable and decays exponentially, for all $x, y \in \mathbb{R}$ and $\lambda \in \Lambda$. However when $n = 2$, both methods are not well suited if one wants to achieve equivalent accuracy to the method used for computing the Evans function. We use the product-integration method, since the weights w_j in (6.15) can be analytically computed as in (6.15), for example. Thus, the $(n-1)$th jump discontinuity of the Green's function g_0 along the diagonal is absorbed in the computation of w_j. Hence, the error convergence will entirely depend on the smoothness of the function hu. Therefore, if a given function $f \in C^{n+1}([a,b])$, then using nth degree polynomial interpolation will

result in an $O(N^{-n-1})$ order of convergence, for uniform mesh x_i (cf. [4, p. 340]). In fact, numerically we have observed that choosing uniformly distributed nodes x_i in the finite domain yields better convergence than considering Gauss–Hermite quadrature rule. Thus, we choose the product-integration and the mapping method over Gauss–Hermite quadrature rule in all our examples.

Remark 6.3. Since we assume that the differential operator $(\mathcal{L}_0 - \lambda\mathrm{id})$ has constant coefficients, the associated integral operator $\mathcal{K}(\lambda)$ is of trace class (cf. Theorem 4.2 or Proposition 4.3 of Chapter 4).

Example 6.1 (Schrödinger equation)**.** We consider the Schrödinger problem [44] given by

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \big(6\phi^2(x) - 1\big)u = \lambda u$$

where $\phi(x) = \mathrm{sech}(x)$ is the steady wave. The essential spectrum for this example is $(-\infty, -1]$. Therefore $\Lambda = \mathbb{C} \setminus (-\infty, -1]$. For $\lambda \in \Lambda$ and $u \in L^2(\mathbb{R})$, the associated integral equation is

$$u = 6\mathcal{K}(\lambda)u,$$

where

$$\mathcal{K}(\lambda)u(x) = \frac{1}{2\sqrt{\lambda+1}} \int_{\mathbb{R}} \phi(x)\mathrm{e}^{-\sqrt{\lambda+1}|x-y|}\phi(y)u(y)\mathrm{d}y.$$

For $\lambda \in \Lambda$, the Fourier transform of the resolvent operator $(\mathrm{d}^2/\mathrm{d}x^2 - \sqrt{\lambda+1}^2)^{-1}$ on $\mathbb{R}$ is $-1/(\xi^2 + \sqrt{\lambda+1}^2)$ for which its inverse transform is $\mathrm{e}^{-\sqrt{\lambda+1}|x|}/2\sqrt{\lambda+1}$. Hence the above integral operator follows.

Our aim in this example is to test the effectiveness of our method. Computing the Fredholm determinant by the trapezoidal rule, the mapping method or the generalised trapezoidal, i.e. equation (6.14) and (6.15), we obtain an $O(N^{-2})$ order of convergence, at the eigenvalue $\lambda = 3$. However, the second degree polynomial interpolation yields an $O(N^{-4})$ order of convergence which is similar to that of the Evans function (see Figure 6.1 (left)). For comparison reasons, we implement a non-adaptive Runge–Kutta method when computing numerically the Evans function $E(\lambda)$. We truncate the infinite domain at $R = \pm 5$. In Figure 6.1 (left), we plot the errors of the Evans function and the Fredholm determinant denoted by $|E_N(\lambda)|$ and $|d_N(\lambda)|$, respectively. Since the eigenvalues $\lambda_0 = 0$ and $\lambda_0 = 3$ of $\mathcal{K}(\lambda)$ are simple, we have for all $\lambda \in \Lambda$,

that

$$|E_N(\lambda)| = |c_N(\lambda)d_N(\lambda)|$$

$$\leqslant c|c_N(\lambda)| \max_{i=1,2}\{\|\mathcal{K}(\lambda)u_i - \mathcal{K}_N(\lambda)u_i\|\},$$

where $|c_N(\lambda)|$ is a nonvanishing analytic function and where u_i are the eigenfunctions corresponding to the eigenvalue $\lambda_0 = 0$ or 3. In particular, when $c_N(\lambda) \to 1$ as $N \to \infty$ (the nonvanishing analytic function connecting the Fredholm determinant and the Evans function $c(\lambda) = 1$), the error in the Evans function denoted by RK4a in the legend of Figure 6.1 (left) and the Fredholm determinant coincide. In Figure 6.1 (left), the legend RK4b corresponds to the error in the Evans function divided by $c(\lambda) = 2\sqrt{\lambda + 1}$. Despite the fact that the RK4 is computationally less expensive than our method, we nevertheless display CPU time versus error, in Figure 6.1 (right).

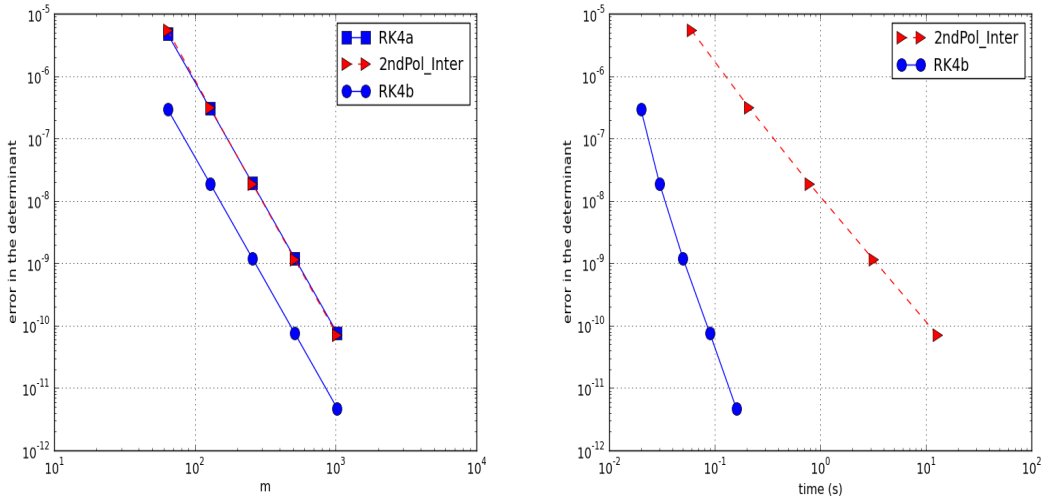

Figure 6.1: Error in the Evans function and the Fredholm determinant versus the discretisation points N (left), and versus CPU time (right), at the eigenvalue $\lambda = 3$.

In the next two examples, our aim is to numerically compute the Fredholm determinant $d(\lambda)$ and the Evans function $E(\lambda)$. In these examples, the coefficients ϕ_i in the perturbation v are given by (4.38). In that case, we integrate by parts. We do not focus on the error analysis in Example 6.2 since it is similar to Example 6.1, i.e. the

new kernel (obtained after integration) has a jump discontinuity in the first derivative, and the corresponding integral operator has simple eigenvalue $\lambda_0 \in [0, 0.02]$ (see Figure 6.2).

Example 6.2 (Boussinesq system [40,52])**.** We consider the 'good' Boussinesq equation given by

$$\lambda^2 u - 2c\lambda \frac{\mathrm{d}u}{\mathrm{d}x} = (1-c^2)\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} - \frac{\mathrm{d}^4 u}{\mathrm{d}x^4} - \frac{\mathrm{d}^2}{\mathrm{d}x^2}(2\phi(x)u) \tag{6.16}$$

where $|c| < 1$ and

$$\phi(x) = \frac{3}{2}(1-c^2)\mathrm{sech}^2\left(\frac{\sqrt{1-c^2}}{2}x\right).$$

Here the essential spectrum is $\sigma_e = \{\lambda \in \mathbb{C}\colon \lambda^2 - i2c\lambda\xi = -(1-c^2)\xi^2 - \xi^4,\ \xi \in \mathbb{R}\}$. Hence $\Lambda = \mathbb{C} \setminus \sigma_e$. The travelling wave ϕ is stable for $1/2 < |c| < 1$ and unstable when $|c| < 1/2$. In Figure 6.2, we plot the Fredholm determinant and the Evans function for $\lambda \in [0, 0.2]$ and $c = 0.4$. The truncation point of the infinite domain is $R = \pm 8$. The coordinate patches are identified by $\mathfrak{i}^- = \{1, 2\}$ and $\mathfrak{i}^+ = \{3, 4\}$ which are chosen as the pivot rows of the matrices Y^- and Y^+ respectively. The eigenvalue λ of equation (6.16) is located at approximately 0.155. $|d_m(\lambda)|$ at the eigenvalue $\lambda \approx 0.155$ is roughly the same as in Example 6.1 since the kernel associated to the Boussinesq problem is similar to the kernel in Example 6.1.

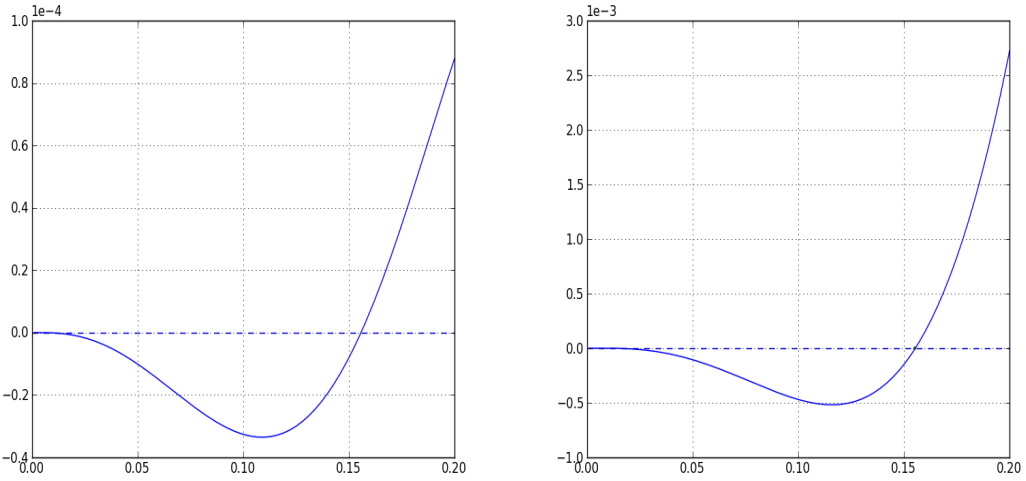

Figure 6.2: Fredholm determinant (left) and Evans function (right) for the Boussinesq equation.

Suppose that the kernel function k is sufficiently smooth. Then product-integration may not be needed if we are seeking only reasonable accuracy. Instead, we can simply apply the regular trapezoidal rule (in a truncated domain) or a Gaussian quadrature on a finite domain (obtained by transformation) to get the desired accuracy. For instance, the kernel function k associated with the 5th order KdV in Example 6.3 is in $C^3(\mathbb{R}^2 \times \mathbb{C}^+)$ and decays exponentially. Therefore mapping a subset $L^2(\mathbb{R})$ to $C\big((-1,1)\big)$ and using Chebyshev quadrature for fixed $x \in (-1,1)$ (a section of the kernel), we expect an $O(N^{-4})$ order of convergence deduced from that of the Chebyshev coefficients of the section $y \mapsto k(x,y,\lambda)$. More generally, if a function is $C^{n-2}\big((-1,1)\big)$, then the order of convergence is $O(N^{-n+1})$ for the Chebyshev quadrature (cf. [18, p. 52] or [22] for the rate of convergence associated with the Chebyshev coefficients and [18, p. 55-56] for the quadrature error). Thus the rate of convergence of the Fredholm determinants is $O(N^{-n+1})$, since the convergence rate of the Nyström method (i.e. $\|\mathcal{K}u - \mathcal{K}_N u\|$, $\mathcal{K}$ an integral operator in $C\big((-1,1)\big)$ and $\mathcal{K}_N$ its approximation) is the same as the underlying quadrature rule for continuous functions (cf. [18]).

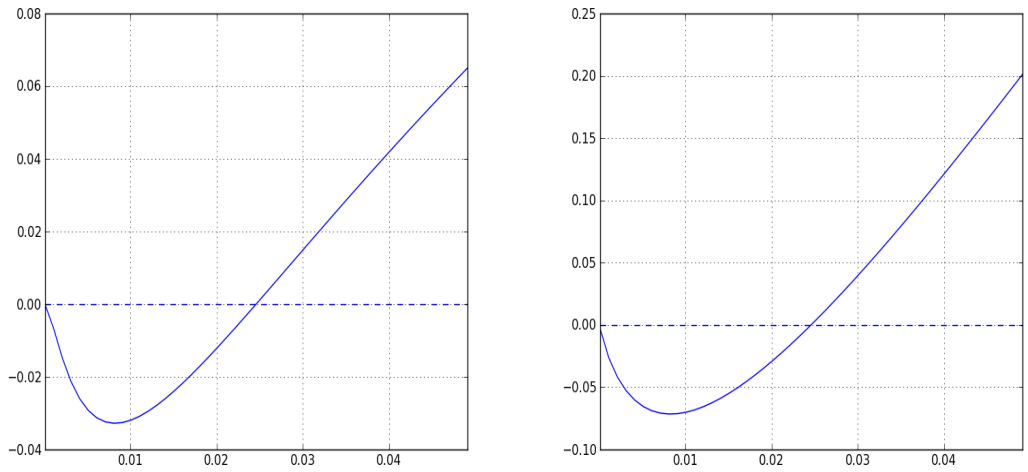

Figure 6.3: Fredholm determinant (left) and the Evans function (right) for the fifth order KdV equation with $q = 10$.

Example 6.3 (Fifth-order KdV equation [14])**.**

$$\frac{\mathrm{d}^5 u}{\mathrm{d}x^5} - \frac{\mathrm{d}^3 u}{\mathrm{d}x^3} + c\frac{\mathrm{d}u}{\mathrm{d}x} - (q+1)\frac{\mathrm{d}}{\mathrm{d}x}(\phi^q(x)u) = \lambda u$$

where

$$c = 4(q+2)(q^2+4q+8)^{-2}$$

$$\phi(x) = \alpha^{1/q}\mathrm{sech}^{4/q}(\beta x)$$

with $\alpha = (q+4)(3q+4)(q+2)(q^2+4q+8)^{-2}/2$ and $\beta = q^2(q^2+4q+8)^{-1}/4$. Here the essential spectrum is $\sigma_e = \{\lambda \in \mathbb{C}\colon \lambda = i(\xi^5+\xi^3+c\xi),\ \xi \in \mathbb{R}\}$, and so $\Lambda = \mathbb{C}\setminus\sigma_e$. For $q \geqslant 5$, the travelling wave ϕ is known to be unstable with real eigenvalue $\mathrm{Re}\,\lambda > 0$ and stable for $q \leqslant 4$. For $q = 10$, the eigenvalue is approximately 0.02457274 (see Figure 6.3). The coordinate patches for the fifth-order KdV equation are identified by $\mathfrak{i}^- = \{2,3,4\}$ and $\mathfrak{i}^+ = \{1,5\}$ which again represent the row pivots of Y^- and Y^+ respectively.

N	RK4	Trapezoidal rule	Domain mapping
256	0.024582699170801733	0.024572650133556081	0.024572769465875954
512	0.024573330975408373	0.024572765920538326	0.024572773336776935
1024	0.024572805577677628	0.024572773115652344	0.024572773578513393

Table 6.1: Eigenvalue of the 5th order KdV equation computed for different value of N and $q = 10$.

The values in Table 6.1 are obtained from calling the `scipy.fsolve`[1] (a root solver) to compute the zeros of the Evans function and the Fredholm determinant with the truncation point $R = \pm 20$. the trapezoidal rule. For comparison, the `scipy.odeint`[2] solver, with relative tolerance 10^{-12} and absolute tolerance 10^{-14}, was used to compute the Evans function leading to the eigenvalue $\lambda = 0.0245727735871733$. eigenvalue is 0.0245726200928363. Theoretically, the rate of convergence of both trapezoidal

[1]scipy is a scientific module for Python, and fsolve is a wrapper around MINPACK's hybrd and hybrj algorithms (a root-finding method)

[2]It uses LSODA from the Fortran library odepack that implements Adam's method for non-stiff problem with default order 12.

rule and mapping method applied to a section of the kernel is at least $O(N^{-2})$ and $O(N^{-4})$ respectively. Accordingly, these rates are those of Nyström methods as well. We observe from Table 6.1 that the trapezoidal rule is more accurate than the RK4 method. Thus one might argue that its rate of convergences is proportional to that of RK4 or the constant of proportionality (in $O(N^{-2})$) for the trapezoidal rule is very small. However, we see from Figure 6.4 (left), where we display the error $|\lambda - \lambda_N|$ versus the number of points N, that the order of convergence of the trapezoidal rule is $O(N^{-4})$. This, in fact, is due to the regularity of the kernel, $C^3(\mathbb{R}^2)$ and the boundedness of the 4th order derivative with respect to the second argument (see [22]). The set of zeros $\{\lambda_N\}_{N\geqslant 1}$ corresponds to both the finite dimensional determinant $d_N(\lambda)$, computed using the trapezoidal rule, and the approximate Evans function. In Figure 6.4 (right) we plot the error $|\lambda - \lambda_N|$ versus the CPU time. It is seen from Figure 6.4 (right) that high accuracy in computing of eigenvalues can be obtained by the use of the trapezoidal rule with minimum effort for $N \leqslant N_0$. In fact, assuming that the eigenvalues $\kappa_j^{\pm}$ are given explicitly, then the effort in forming the determinant in (6.12) is $\mathcal{O}(N(n-k)^2k^2)$ when applying the Riccati-RK4. While applying the trapezoidal rule, the finite dimensional determinant $d_N(\lambda)$ is $\mathcal{O}(N^2 + n^\alpha)$, where n^α is the complexity for solving the linear systems (4.41) of Chapter 4.

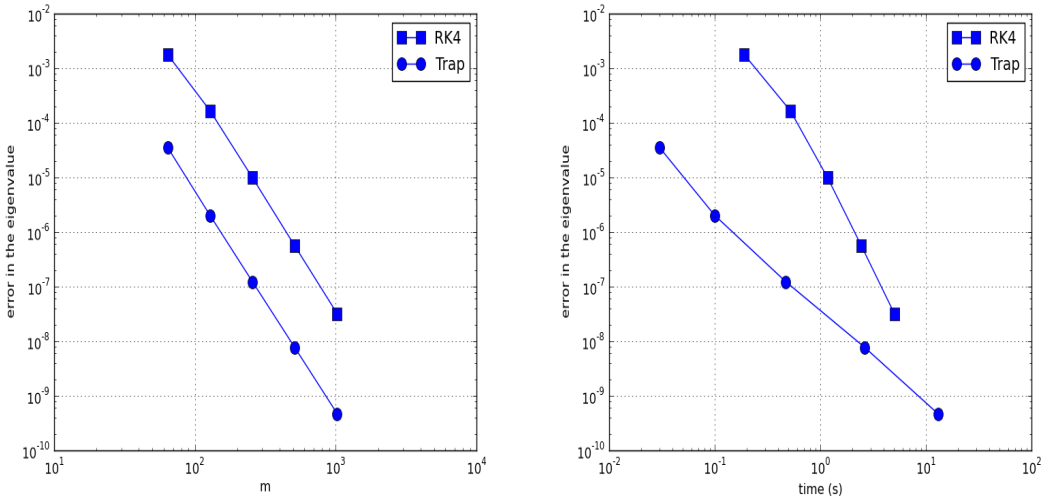

Figure 6.4: Error in the eigenvalue versus discretisation points N (left), and versus the CPU time (right).

6.4 Concluding remarks

Depending on accuracy, we favour product-integration method over other quadrature methods. This is because if the function $h \times u$ is sufficiently smooth then high degree polynomial interpolation can be used for the approximation. As consequence, improved convergence than that of RK4 used for computing Evans function can be achieved unless one implements a Runge–Kutta method of order equal to that of the product-integration method. When it comes to CPU time, product-integration/trapezoidal rule is inferior to Runge–Kutta method for some range of discretisation points, but also there is a range in which it is faster (see Figure 6.4). Nevertheless, by converting the eigenvalue problem into an integral eigenvalue problem, we have the following advantages:

1. Partially solving the problem;

2. Any $\lambda \in \Lambda$ satisfying $\det_p\big(\mathrm{id} + \mathcal{K}(\lambda)\big) = 0$ is an eigenvalue of the corresponding differential operator with algebraic multiplicity equal to that the eigenvalue -1;

3. We do not encounter the numerical stiffness problem. This is because the Green's function is the projection of the evolution (or propagator) onto the appropriate subspaces which are associated with a single exponential growth and decay modes.

The effort in computing the Fredholm determinants can be considerably reduced, if adaptive algorithms are implemented in choosing the correct quadrature points. The problem is then we need to find a suitable residual to implement 'adaptive' steps. If both the numerical Fredholm determinant and the Evans function are coded in a compiling language, then the effort of both methods is the same.

Chapter 7

Conclusion and future work

The aim of this thesis was to theoretically and numerically investigate the stability of travelling wave solutions by employing Fredholm determinants. During our investigation, several results were obtained/improved which we now recall.

7.1 Conclusion

Chapter 2 and 3 recall some essentials about compact operators and Fredholm determinants and introduce the Evans function as well as the considered problem.

In Chapters 4, we have shown that for a class of eigenvalue problems, the associated integral operators are of trace class, in particular for constant coefficient differential operators corresponding to the unperturbed eigenvalue problem. Through the determinant of the matrix transmission coefficient, we have established the connection between the Fredholm determinant associated with trace class operators and the Evans function, and then extended it to any integral operator in the Schatten–von Neumann class. This has led to connecting the Evans function and the determinant of the linear differential operator associated with the eigenvalue problem. Furthermore we have shown how to construct the Fredholm determinant associated with the linear stability of front waves, and hence its connection with the Evans function of the original problem follows. Based on the connection for the one dimensional problem, one can extend it to the higher dimensional context. One way this is accomplished, it is to convert the higher dimensional problem to a one dimensional one. This can

be achieved by projecting a chosen direction associated with the higher dimensional problem onto a finite dimensional basis, for example by Fourier transform (Gesztesy et al [29]) (e.g projecting the transverse direction of travelling wave problems in a infinite cylinder).

Chapter 5 has dealt mainly with the numerical evaluation of the modified or regularised Fredholm determinants, for integral operators depending linearly on the spectral parameter λ. We have proved the uniform convergence of the modified Fredholm determinants. Thus we have generalised the uniform convergence result for integral operators with continuous kernels due to Bornemann. Moreover, we have shown that the rate of convergence is different when evaluating the modified Fredholm determinants at the resolvent set and at the spectrum. We have also provided numerical examples from which we have observed exactness when evaluating the determinant at an eigenvalue. Consequently, this exactness implies that computing the Fredholm determinants is nothing other than an interpolation in which the zeros are the interpolating points. Furthermore, we have proposed a method to compute higher order determinants, in particular for integral operators belonging to the Schatten–von Neumann class $\mathfrak{I}_3$ and $\mathfrak{I}_4$.

In Chapter 6, we have turned our attention to the case of Fredholm determinants associated with integral operators that do not depend linearly on λ. In our case, this arises when computing the Fredholm determinant associated with linear stability of travelling waves. Numerically we have compared both accuracy and time execution of the Fredholm determinant and the Evans function. This has led us to the following conclusion: depending on the smoothness of the Green's function, high accuracy is achievable within or outside the range in which the computation of the Fredholm determinants requires less effort. However for the method considered in this thesis, the numerical computation of the Evans function requires minimum effort but is less accurate, depending on the degree of the problem and the order of the Runge–Kutta method being implemented.

7.2 Future work

In multidimensional travelling wave problems, besides projection to create an algebraic eigenvalue problem approximation, there are not many approaches. A future direction would be to use the (infinite dimensional) centre manifold which might reduce the high dimensionality of the problem, and then investigate the relation between the Fredholm determinant and the Evans function associated with the lower dimensional problem. Since the modified Fredholm determinants extend naturally to higher dimension, a connection with the generalised Evans function defined as the determinant bundle over the Fredholm Grassmannian space (cf. Deng et al. [19]) is another direction to pursue. The major problem in this approach is the construction of the Green's function for the corresponding integral operator.

To our knowledge, the generalised Evans function due to Deng et al. has not been yet computed numerically. Hence this is a direction to consider together with the numerical computation of the modified Fredholm determinants. In the one dimensional case, improving the complexity effort in computing the Fredholm determinant by taking advantages on the properties of the Green's function is an interesting direction for future investigation. Computing resonances for travelling wave problems using the Fredholm determinants is a prospect of future research as well.

Appendix A

Exterior Product

Let V be a finite dimensional vector space over the field of scalars $\mathbb{F}$.

Definition A.1. An *alternating multilinear form* of degree k on a vector space V is a map $f\colon V \times V \cdots \times V \to \mathbb{F}$ such that, for $\mathbf{u}_i, \mathbf{v}_1, \mathbf{v}_2 \in V$ and $\alpha_1, \alpha_2 \in \mathbb{F}$,

- $f(\mathbf{u}_1, \ldots, \mathbf{u}_i, \ldots, u_j, \ldots, \mathbf{u}_k) = -f(\mathbf{u}_1, \ldots, \mathbf{u}_j, \ldots, \mathbf{u}_i, \ldots, \mathbf{u}_k)$
- $f(\alpha_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2, \mathbf{u}_2, \ldots, \mathbf{u}_n) = \alpha_1 f(\mathbf{v}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n) + \alpha_2 f(\mathbf{v}_2, \mathbf{u}_2, \ldots, \mathbf{u}_n)$
- $f(\mathbf{u}_1, \ldots, \mathbf{u}_i, \ldots, \mathbf{u}_j, \ldots, \mathbf{u}_k) = 0$, if $i = j$.

The set of all alternating multilinear forms on V is a vector space.

Example A.1. Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be column vectors in $V = \mathbb{R}^n$. Then

$$f(\mathbf{u}_1, \ldots, \mathbf{u}_n) = \det_{\mathbb{R}^n}\begin{pmatrix}\mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_n\end{pmatrix}$$

is an alternating multilinear form of degree n.

Definition A.2. The *k-th exterior power* $\bigwedge^k V$ of a finite dimensional vector space is the dual space of the vector space of alternating multilinear forms of degree k on V. Elements of $\bigwedge^k V$ are called k-vectors or k-forms.

Definition A.3. Given $\mathbf{u}_1, \ldots, \mathbf{u}_k \in V$, the *exterior product* $\mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \cdots \wedge \mathbf{u}_k \in \bigwedge^k V$ is the linear map to $\mathbb{F}$ which, on an alternating multilinear form M takes the values

$$(\mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \cdots \wedge \mathbf{u}_k)(f) = f(\mathbf{u}_1, \ldots, \mathbf{u}_k).$$

If the dimension of the vector space V is n and $\{\mathbf{e}_i\}_{i=1,\dots,n}$ is a basis of V, then the set

$$\{\mathbf{e}_{i_1} \wedge \mathbf{e}_{i_2} \wedge \cdots \wedge \mathbf{e}_{i_k} : 1 \leqslant i_1 < i_2 < \cdots < i_k \leqslant n\}$$

is a basis of $\bigwedge^k V$. The dimension of the vector spaces $\bigwedge^k V$ is

$$\binom{n}{k}.$$

If $k = n$ then $\bigwedge^n V$ is a one dimensional vector space. By convention $\bigwedge^0 V = \mathbb{F}$.

Proposition A.1. *The exterior product $\boldsymbol{u}_1 \wedge \boldsymbol{u}_2 \wedge \cdots \wedge \boldsymbol{u}_k$ of k vectors $\boldsymbol{u}_i \in V$ vanishes if and only if the vectors are linearly dependent.*

Definition A.4. A k-form is *decomposable* if it is wedge product between k linearly independent vectors in V.

Let $\mathbb{F} = \mathbb{C}$ and $V = \mathbb{C}^n$. The *inner product* on V, represented by $\langle \cdot, \cdot \rangle$, is the map from $V \times V$ to $\mathbb{C}$ satisfying, for all $\mathbf{u}_j \in V$ and $\alpha_j \in \mathbb{C}$ $(j = 1, 2, 3)$, the following

1. $\langle \alpha_1 \mathbf{u}_1 + \alpha_2 \mathbf{u}_2, \mathbf{u}_3 \rangle = \alpha_1 \langle \mathbf{u}_1, \mathbf{u}_3 \rangle + \alpha_2 \langle \mathbf{u}_2, \mathbf{u}_3 \rangle$;
2. $\langle \mathbf{u}_1, \alpha_2 \mathbf{u}_2 + \alpha_3 \mathbf{u}_3 \rangle = \bar{\alpha}_2 \langle \mathbf{u}_1, \mathbf{u}_2 \rangle + \bar{\alpha}_3 \langle \mathbf{u}_1, \mathbf{u}_3 \rangle$;
3. $\langle \mathbf{u}_1, \mathbf{u}_1 \rangle \geqslant 0$ and $\langle \mathbf{u}_1, \mathbf{u}_1 \rangle = 0$ implies that $u_1 = 0$;
4. $\langle \mathbf{u}_1, \mathbf{u}_2 \rangle = \overline{\langle \mathbf{u}_2, \mathbf{u}_1 \rangle}$.

The inner product $[\![\cdot, \cdot]\!]_k$ of two decomposables k-forms

$$\mathbf{U} = \mathbf{u}_1 \wedge \ldots \wedge \mathbf{u}_k \quad \text{and} \quad \mathbf{V} = \mathbf{v}_1 \wedge \ldots \wedge \mathbf{v}_k$$

on $\bigwedge^k \mathbb{C}^n$ with $\mathbf{u}_i, \mathbf{v}_j \in \mathbb{C}^n$ is defined by

$$[\![\mathbf{U}, \mathbf{V}]\!]_k = \det{}_{\mathbb{C}^k} \Big(\big(\langle \mathbf{u}_i, \mathbf{v}_j \rangle \big)_{i,j=1}^{k} \Big).$$

The vector spaces $\bigwedge^k \mathbb{C}^n$ and $\bigwedge^{n-k} \mathbb{C}^n$ are isomorphic and the natural isomorphism is given by the *Hodge star operator* $\star$. Fixing an orientation, the Hodge star is a map from $\bigwedge^k \mathbb{C}^n$ to $\bigwedge^{n-k} \mathbb{C}^n$ (vice versa), defined, for any $\mathbf{U} \in \bigwedge^k \mathbb{C}^n$, by

$$\star \mathbf{U} \in \bigwedge^{n-k} \mathbb{C}^n.$$

The isomorphism of the vector spaces $\bigwedge^k \mathbb{C}^n$ and $\bigwedge^{n-k} \mathbb{C}^n$ is then given, for any $\mathbf{U} \in \bigwedge^k \mathbb{C}^n, \mathbf{V} \in \bigwedge^{n-k} \mathbb{C}^n$, by

$$\mathbf{U} \wedge \mathbf{V} = [\![\mathbf{U}, \star\mathbf{V}]\!]_k \mathcal{V},$$

where $\mathcal{V} = \mathbf{e}_1 \wedge \ldots \wedge \mathbf{e}_n \in \bigwedge^n \mathbb{C}^n$ is a volume form, and $\{\mathbf{e}_i\}_{i=1\ldots n}$ is a basis for $\mathbb{C}^n$.

Appendix B

Matrices S_l and S_r

$$S_l = \begin{pmatrix} 1 & 1 & -1 & 1 & \cdots & (-1)^n \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & -\frac{1}{2} & 0 & \cdots & 0 \\ 0 & \frac{1}{4} & 0 & -\frac{1}{4} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{2(n-1)} & 0 & -\frac{1}{2(n-1)} \\ 0 & 0 & \cdots & 0 & \frac{1}{2n} & 0 \end{pmatrix}$$

$$S_r = \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & -1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & -1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & -\frac{1}{2} & 0 & \cdots & 0 \\ 0 & \frac{1}{4} & 0 & -\frac{1}{4} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{2(n-1)} & 0 & -\frac{1}{2(n-1)} \\ 0 & 0 & \cdots & 0 & \frac{1}{2n} & 0 \end{pmatrix}$$

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